Supplementary Information (SI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2026

Supplementary Information

Bidentate bis(NHC-carboxylate) palladium and nickel complexes for the hydrosilylative reduction of carbonyl compounds.

Jorge Sanz-Garrido,[a] Carlos J. Carrasco,[b] Camino Gonzalez-Arellano,[a] Francisco Montilla,[b] Agustín Galindo,*[b] Juan C. Flores *[a]

[a] *Departamento de Química Orgánica y Química Inorgánica. Instituto de Investigación Química "Andrés M. del Río", Universidad de Alcalá. Campus Universitario, 28805 Alcalá de Henares, Madrid, Spain.*

[b] *Departamento de Química Inorgánica, Facultad de Química, Universidad de Sevilla, 41071, Sevilla, Spain.*

Table of Contents

General considerations

All reactions were conducted under argon atmosphere using standard Schlenk and dry-box techniques. The reagents were purchased from commercial sources and used as received. Solvents were purchased from commercial sources and were dried using standard methods,[1] distilled and stored in inert atmosphere. Argon N-50 was purchased from Abelló-Linde. Chromatography was performed on silica gel 40 – 63 μm (230-400 mesh) for the scope of the reaction. Deuterated chloroform for NMR spectroscopy was used as received, deuterated DMSO was stored as received over molecular sieves, and deuterated toluene was dried with sodium, distilled, and stored over molecular sieves. NMR spectra were recorded at room temperature using Varian Mercury Plus-300, Varian NMR System 500, Bruker 400 Ultrashield or Bruker AVANCE Neo 400 Nanobay spectometers. When required, monodimensional ^{1}H-NOE and bidimensional ^{1}H–^{13}C HSQC, ^{1}H–^{13}C HMBC, or ^{1}H-^{1}H COSY, experiments were performed for unequivocal assignment of resonances for the new compounds. Chemical shifts (δ, parts per million) are quoted relative to $SiMe_4$ and were measured by internal referencing to residual signals of the deuterated solvents. Coupling constants (J) are given in Hertz. High-resolution mass spectra were conducted in an Agilent LC/MS-TOF 6210 mass spectrometer at the Chemical Research Support Centre of the University of Alcalá. Polarimetry was carried out using a Perkin-Elmer 341 polarimeter and the measurements were made at 20 ºC temperature in ethanol or dichloromethane (concentration of ca. 0.100 g/100 mL). The progress of the catalytic reactions was determined using an Agilent GC-MS turbo system (5975-7820A model) equipped with an autoinjector, and using an Agilent 19091S-433 HP-5MS capillary column (30 m × 0.25 mm i.d., 0.25 μm df) under the following conditions injector and detector temperatures: 250 °C and 230 °C, respectively, oven temperature program: 2.5 min initial isotherm at 50 ºC, ramp up to 120 °C at 4 °C/min, and ramp up to 220 °C at 25 °C/min, solvent delay of 2.5 min. The imidazolium salts (Figure S1) were synthetized following procedures already described.[2]

[1] W. L. F. Armarego, C. L. Lin Chai, Purification of Laboratory Chemicals, 6th ed., Elsevier, Oxford, 2009.
[2] J. Sanz-Garrido, A. Martin, C. González-Arellano, J. C. Flores, *Dalton Trans.* **2024**, *53*, 1460–1468.

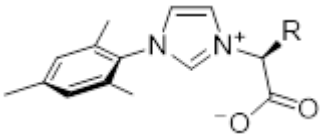
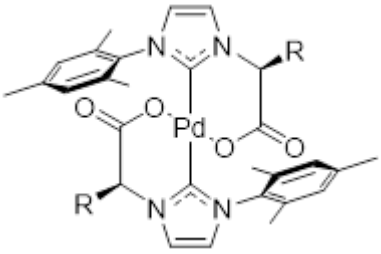


Figure S1. Imidazolium salts (**MesAA**)H.

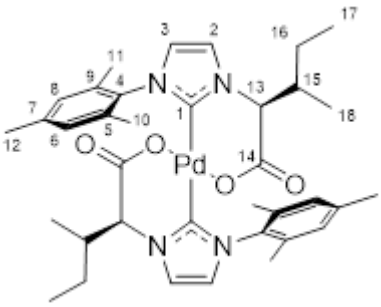
The ^{1}H-NMR spectra of the Ni complexes **Leu$_2$Ni**, **ILe$_2$Ni** and **Phe$_2$Ni** is consistent with those reported in the bibliography.[2] The numbering in the figure for each compound below is for NMR assignment purposes only; they are not intended to be locants. Abbreviations: ACN (acetonitrile), DCM (dichloromethane).

Synthesis of Pd complexes: Procedure for synthesis of the complex



To a schlenk under inert atmosphere it is added the corresponding imidazolium salt (2 equiv) and Ag_2O (2 equiv) and dry DCM (0.1 M), and the mixture is stirred at room temperature overnight protected from the light. The crude is filtered *via* canula to another schlenk containing a solution of $Pd(OAc)_2$ (1 equiv) in dry DCM (0.1 M) and it is stirred at room temperature overnight protected from the light. The solution is filtered, evaporated and the resulting solid washed with pentane.

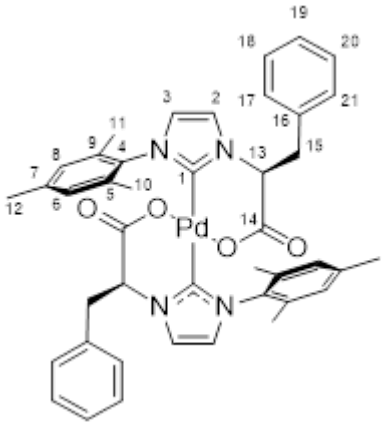
ILe$_2$Pd. bis(1-((*L*)-isoleuci-*N*-yl)-3-mesityl-1*H*-imidazole-2-ylidene)palladium(II)



The product is obtained as a light brown solid (90 mg, 51%).

^{1}H NMR (500 MHz. $CDCl_3$) δ = 7.03 (s; 1H; 8); 6.94 (s; 1H; 6); 6.90 (d; *J* = 1.8; 1H; 3); 6.66 (d; *J* = 1.8 Hz; 1H; 2); 4.10 (d; *J* = 10.5 Hz; 1H; 13); 3.47 – 3.34 (m; 1H; 15); 2.33 (s; 3H; 12); 2.14 (s; 3H; 10); 1.95 (s; 3H; 11); 1.42 – 1.34 (m; 1H; 16); 1.16 – 1.10 (m; 1H; 16); 1.09 (d; *J* = 6.8; 3H; 18); 0.94 (t; *J* = 7.4; 3H; 17). ^{13}C{^{1}H} NMR (126 MHz. $CDCl_3$) δ = 171.7 (14); 163.5 (1); 138.8 (7); 136.1 (9); 134.8 (4); 134.1 (5); 129.0 (8); 128.8 (6); 121.9 (2); 121.9 (3); 72.6 (13); 41.9 (15); 25.6 (16); 21.4 (12); 18.3 (10); 17.3 (11); 15.8 (18); 11.1 (17). Exact mass spectrometry: HRMS (ESI/TOF. positive ions. ACN). For $C_{36}H_{47}N_4O_4Pd$ (M+H) m/z calculated: 705.2632; m/z found: 705.2650. For $C_{38}H_{50}N_5O_4Pd$ (M+H+ACN) m/z calculated: 746.2898; m/z found: 746.2913. Optical activity**:** $[\alpha]^{20}_{D}$ = -264 (C = 0.037 in DCM).

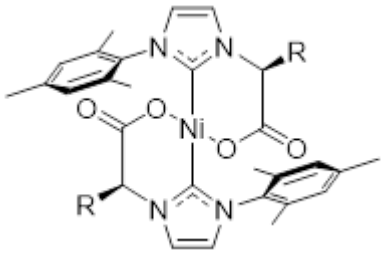
Phe$_2$Pd. bis(1-((*L*)-phenylalanin-*N*-yl)-3-mesityl-1*H*-imidazole-2-ylidene)palladium(II)



The product is obtained as a light brown solid (64 mg, 33%).

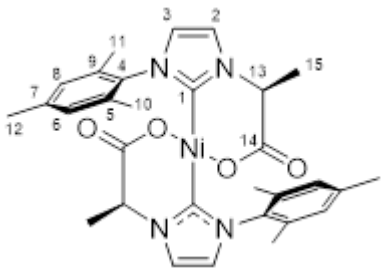
^{1}H NMR (500 MHz. $CDCl_3$) δ = 7.27 – 7.20 (m; 3H; 19, 18, 20); 7.14 (dd; *J* = 7.7, 1.7; 2H; 17, 21); 7.03 (s; 1H; 6); 6.91 (s; 1H; 8); 6.47 (d; *J* = 1.8; 1H; 3); 6.30 (d; *J* = 1.9; 1H; 2); 4.73 (dd; *J* = 11.3, 4.2; 1H; 13); 4.21 (dd; *J* = 13.7 and 11.4; 1H; 15); 3.64 (dd; *J* = 13.6, 4.2; 1H; 15); 2.32 (s; 3H; 12); 2.14 (s; 3H; 11); 2.12 (s; 3H; 10). ^{13}C{^{1}H} NMR (126 MHz. $CDCl_3$) δ = 171.9 (14); 163.9 (1); 138.9 (7); 136.7 (16); 136.1 (5); 134.8 (4); 134.5 (9); 129.1 (17, 21); 129.1 (6); 128.9 (18, 20); 128.7 (8); 127.3 (19); 121.7 (3); 121.1 (2); 68.6 (13); 42.0 (15); 21.4 (12); 18.2 (11); 17.9 (10). Exact mass spectrometry: HRMS (ESI/TOF. positive ions. ACN). For $C_{42}H_{43}N_4O_4Ni$ (M+H) m/z calculated: 773.2314; m/z found: 773.2345. For $C_{44}H_{46}N_5O_4Pd$ (M+H+ACN) m/z calculated: 814.2579; m/z found: 814.2606. Optical activity: $[\alpha]^{20}_D$ = -324 (C = 0.039 in DCM).

Synthesis of Ni complexes: Procedure for synthesis of the complex



To a schlenk under inert atmosphere it is added diisopropylamine (3 equiv) and dry THF (0.1 M), it is cooled to -78 ºC, Li*n*Bu (1.6 M in hexanes) (3 equiv) is added, the mixture is stirred 10 min at that temperature, let to reach room temperature, stirred 10 min and cooled again to -78 ºC. The resulting LDA solution is added *via* canula to a schlenk containing a suspension of the corresponding imidazolium salt (2 equiv) in dry THF (0.1 M) at -78 ºC. Once the addition is completed, the mixture is let to reach room temperature and stirred for 10 minutes and cooled again to -78 ºC. The carbene solution is then added *via* canula to a schlenk containing a suspension of [$NiBr_2$(dme)] (1 equiv) in dry THF (0.1 M) at -78 ºC, the resulting solution is let to reach room temperature and stirred for 2 h. The volatiles are evaporated, and the crude product is purified through chromatography column in silica using AcOEt as eluent.

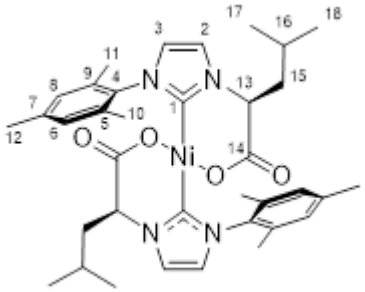
Ala$_2$Ni. bis(1-((*L*)-alan-*N*-yl)-3-mesityl-1*H*-imidazole-2-ylidene)nickel(II)



The product is characterized without purification.

^{1}H NMR (400 MHz. DMSO-d_6) δ = 7.46 (s; 2H; 2); 7.39 (s; 4H; 3, 6); 7.05 (s; 2H; 8); 3.84 (q; *J* = 6.8 Hz; 2H; 13); 2.41 (s; 6H; 12); 2.12 (s; 6H; 10); 1.61 (s; 6H; 11); 1.34 (d; *J* = 6.9 Hz; 6H; 15). ^{13}C{^{1}H} NMR (101 MHz. DMSO-d_6) δ = 170.8 (14); 160.4 (1); 139.3 (7); 137.7 (5); 134.7 (4); 133.8 (9); 129.4 (6); 128.8 (8); 124.0 (2); 119.1 (3); 58.6 (13); 20.5 (12); 18.0 (10); 17.8 (11); 13.8 (15). Exact mass spectrometry HRMS (ESI/TOF. positive ions. ACN). For $C_{30}H_{35}N_4O_4Ni$ (M+H) m/z calculated: 573.2012; m/z found: 573.2004.

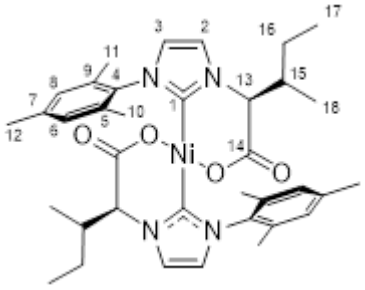
Leu$_2$Ni. bis(1-((*L*)-leucin-*N*-yl)-3-mesityl-1*H*-imidazole-2-ylidene)nickel(II) [2]



The product is obtained as a yellow solid (52%).

^{1}H NMR (500 MHz. DMSO-d_6) δ = 7.50 (s; 2H; 2); 7.09 (s; 2H; 3); 7.04 (s; 2H; 6); 6.85 (s; 2H; 8); 4.40 (t; *J* = 7.6 Hz; 2H; 13); 3.19 (s; 2H; 15); 2.46 (s; 2H; 15); 2.34 (s; 6H; 10); 2.26 (s; 6H; 12); 1.85 (s; 6H; 11); 1.59 (s; 2H; 16); 1.04 (d; *J* = 5.7 Hz; 6H; 18); 1.01 (d; *J* = 6.5 Hz; 6H; 17).

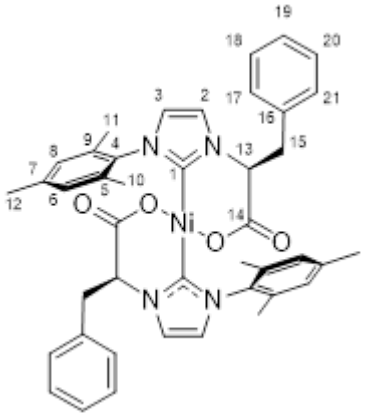
lLe$_2$Ni. bis(1-((*L*)-isoleucin-*N*-yl)-3-mesityl-1*H*-imidazole-2-ylidene)nickel(II) [2]



The product is obtained as a yellow solid (55%).

^{1}H NMR (500 MHz. DMSO-d_6) δ = 7.48 (d; *J* = 1.7 Hz; 2H; 2); 7.10 – 7.00 (m; 4H; 3, 6); 6.82 (s; 2H; 8); 4.21 (s; 2H; 15); 3.94 (d; *J* = 10.1 Hz; 2H; 13); 2.39 (s; 6H; *10*); 2.26 (s; 6H; *12*); 1.79 (s; 6H; *11*); 1.56 – 1.45 (m; 2H; 16); 1.25 (d; *J* = 44.2 Hz; 2H; 16); 1.09 (d; *J* = 6.6 Hz; 6H; 18); 0.98 (t; *J* = 7.4 Hz; 6H; 17).

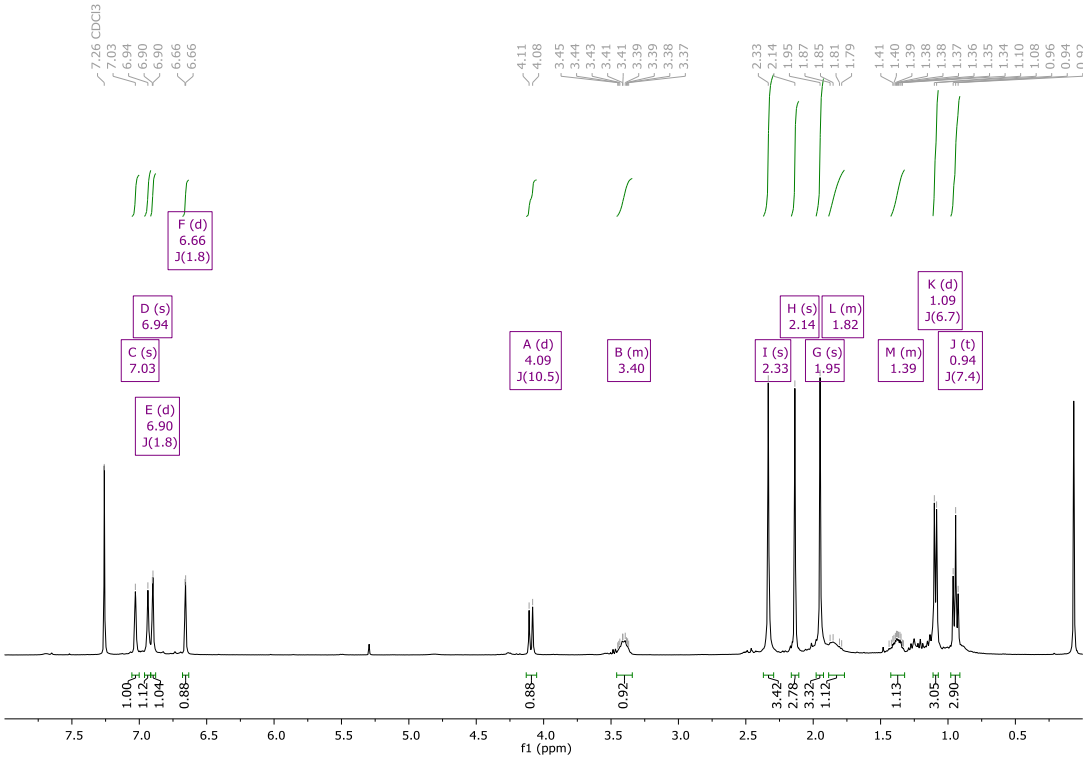
Phe$_2$Ni. bis(1-((*L*)-phenylalan-*N*-yl)-3-mesityl-1*H*-imidazole-2-ylidene)nickel(II) [2]



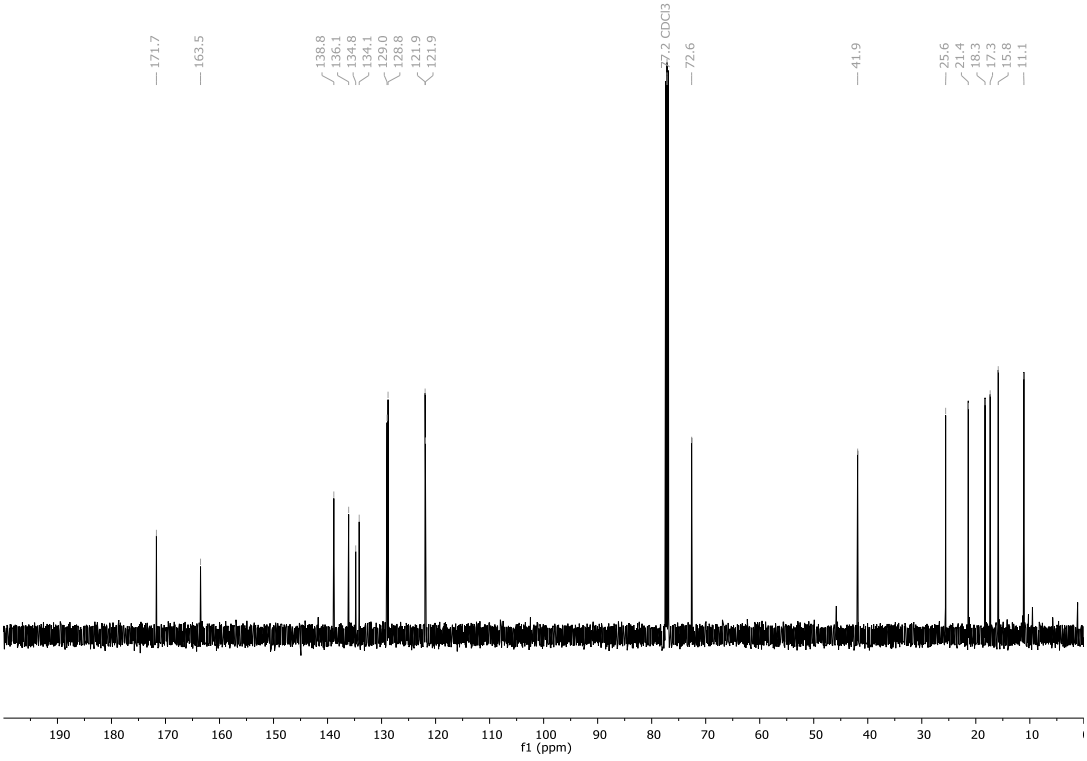
The product is obtained as a yellow solid (51%).

^{1}H NMR (500 MHz. DMSO-d_6) δ = 7.24 (s; 5H; 17-21); 7.04 (s; 1H; 6); 6.91 (s; 1H; 3); 6.87 (s; 1H; 8); 6.81 (br s; 1H; 2); 4.84 (br s; 1H; 15); 4.58 (dd; *J* = 10.4; 5.3 Hz; 1H; 13); 3.94 (d; *J* = 10.4 Hz; 1H; 15); 2.36 (br s; 3H; 11); 2.24 (s; 3H; 12); 1.94 (s; 3H; 10).

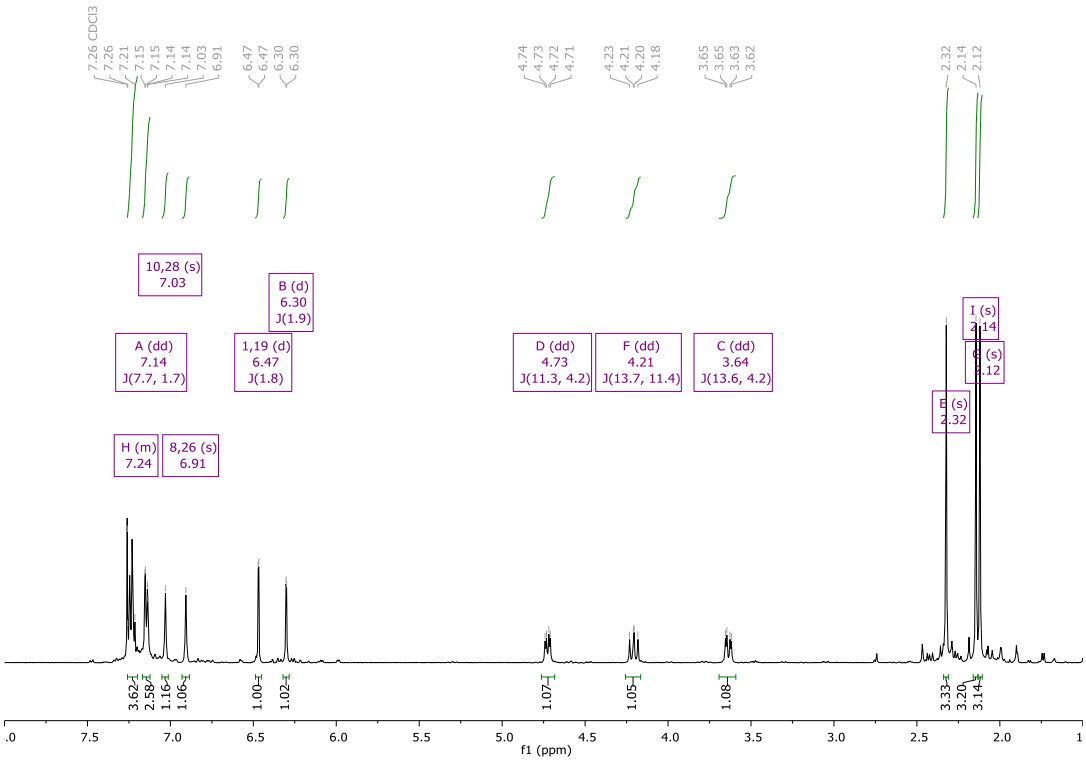
NMR spectra of metal complexes



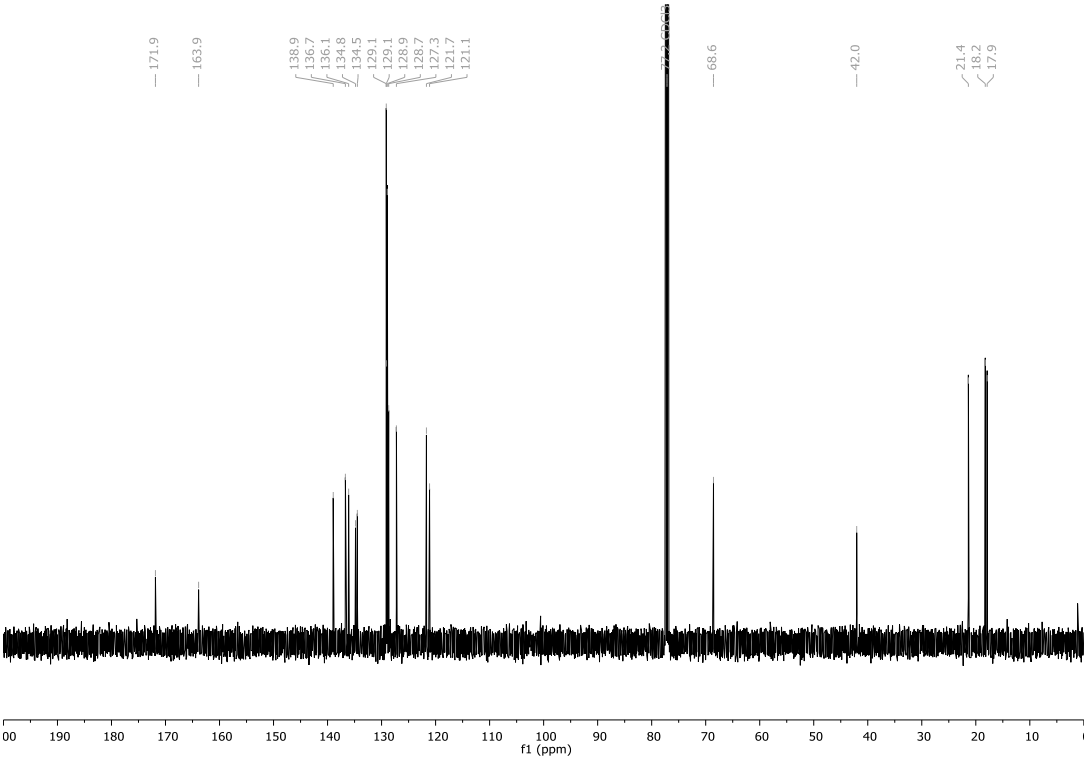
Spectrum S1. ^{1}H NMR spectrum of **ILe$_2$Pd** in $CDCl_3$.



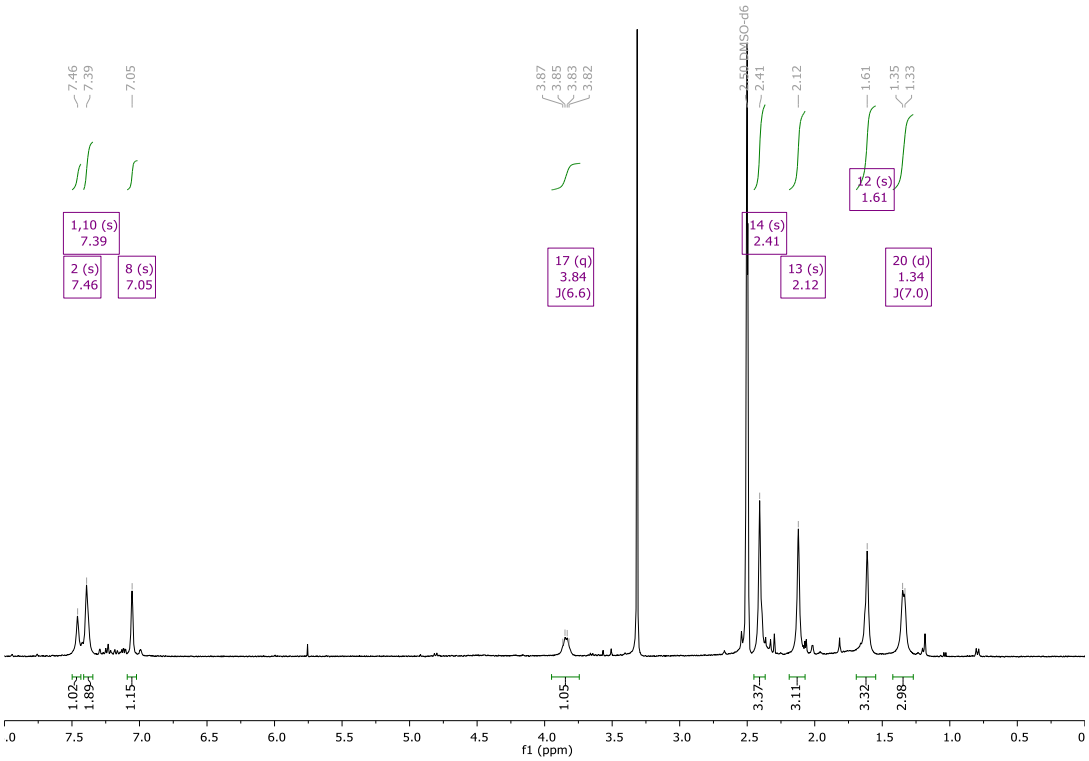
Spectrum S2. $^{13}C\{^{1}H\}$ NMR spectrum of **ILe$_2$Pd** in $CDCl_3$.



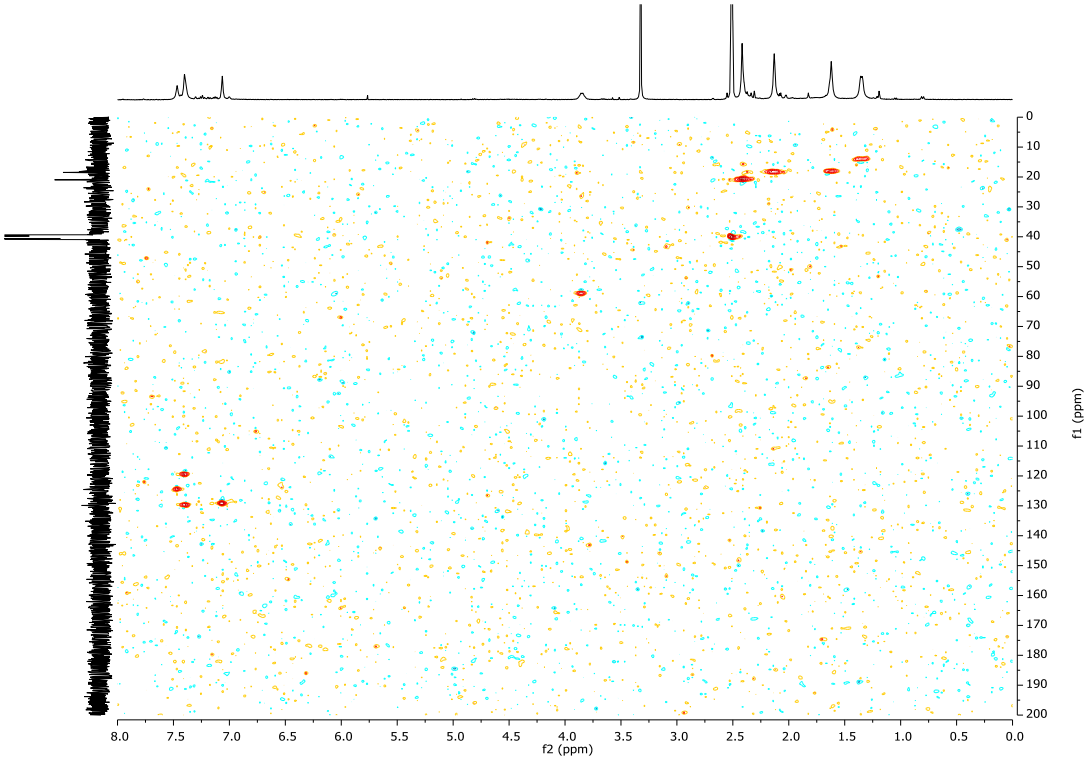
Spectrum S3. ^{1}H NMR spectrum of **Phe$_2$Pd** in $CDCl_3$.



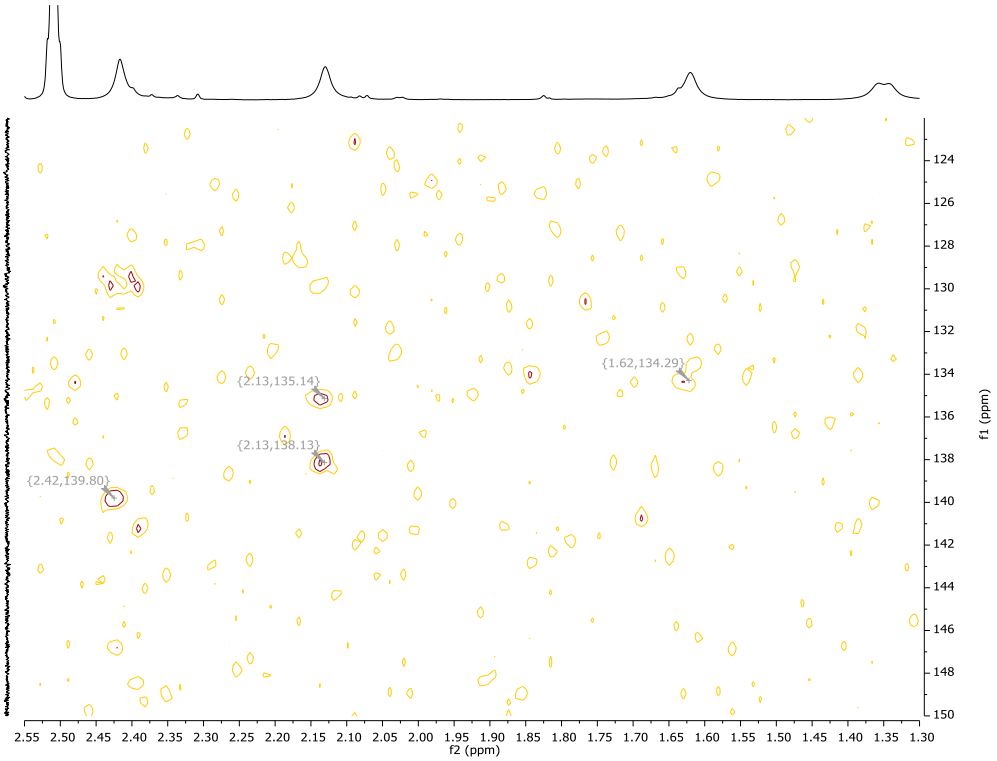
Spectrum S4. ^{13}C{^{1}H} NMR spectrum of **Phe$_2$Pd** in $CDCl_3$.



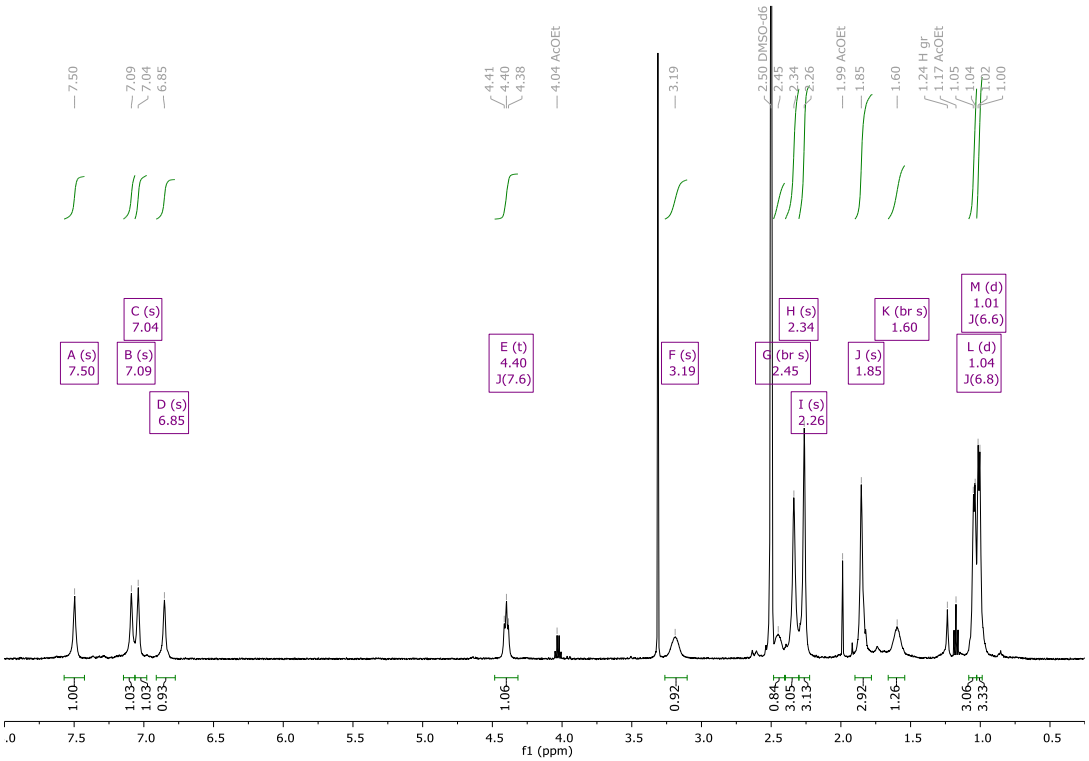
Spectrum S5. ^{1}H NMR spectrum of **Ala$_2$Ni** in DMSO-d_6.



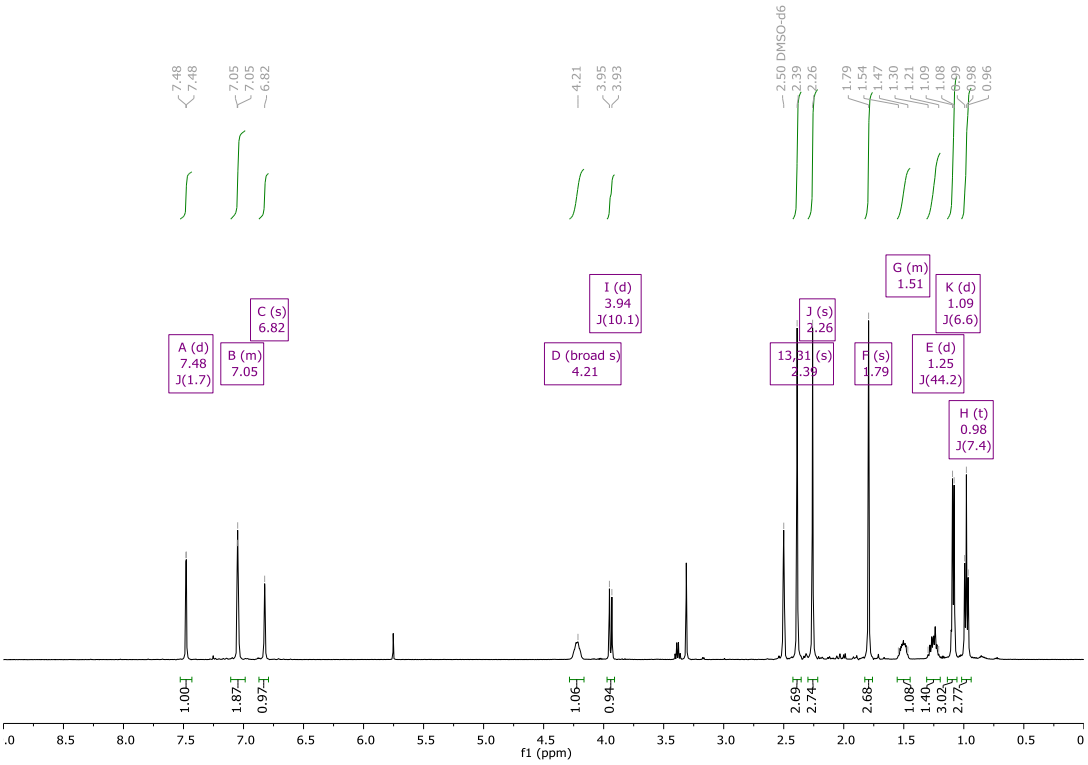
Spectrum S6. ^{1}H-^{13}C HSQC NMR spectrum of **Ala$_2$Ni** in DMSO-d_6.



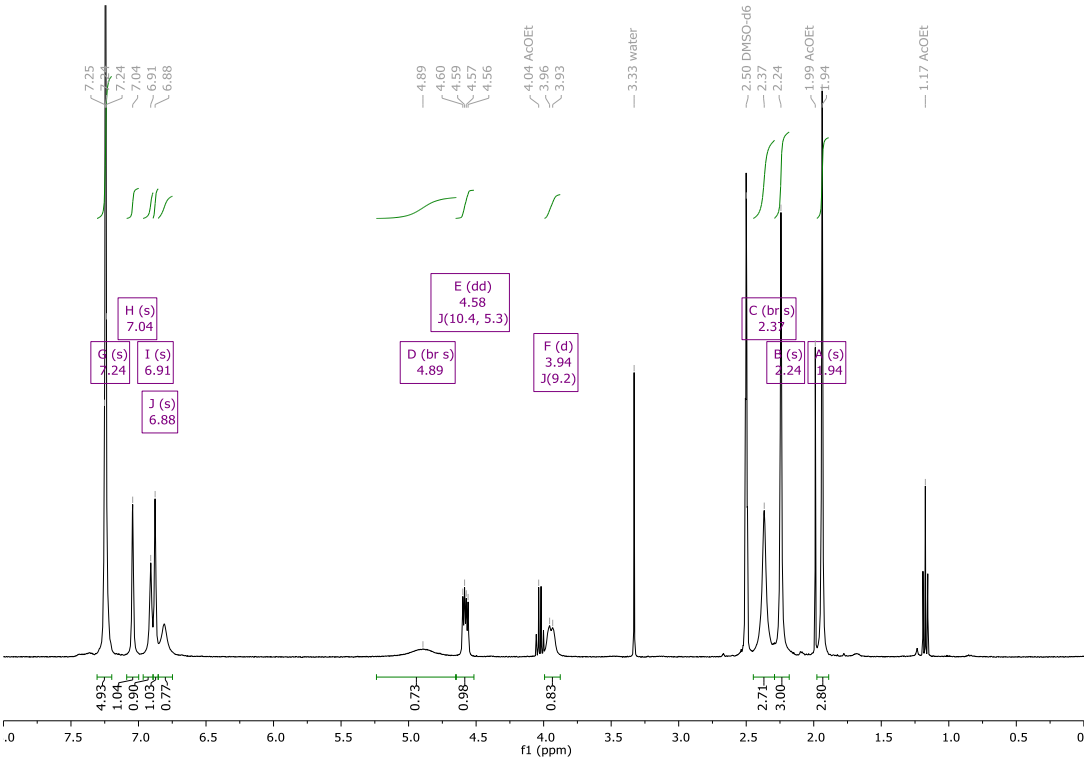
Spectrum S7. Expansion of the ^{1}H-^{13}C HMBC NMR spectrum of **Ala$_2$Ni** in DMSO-d_6 showing the region for the methyl groups of the mesityl rings.



Spectrum S8. ^{1}H NMR spectrum of **Leu$_2$Ni** in DMSO-d_6.

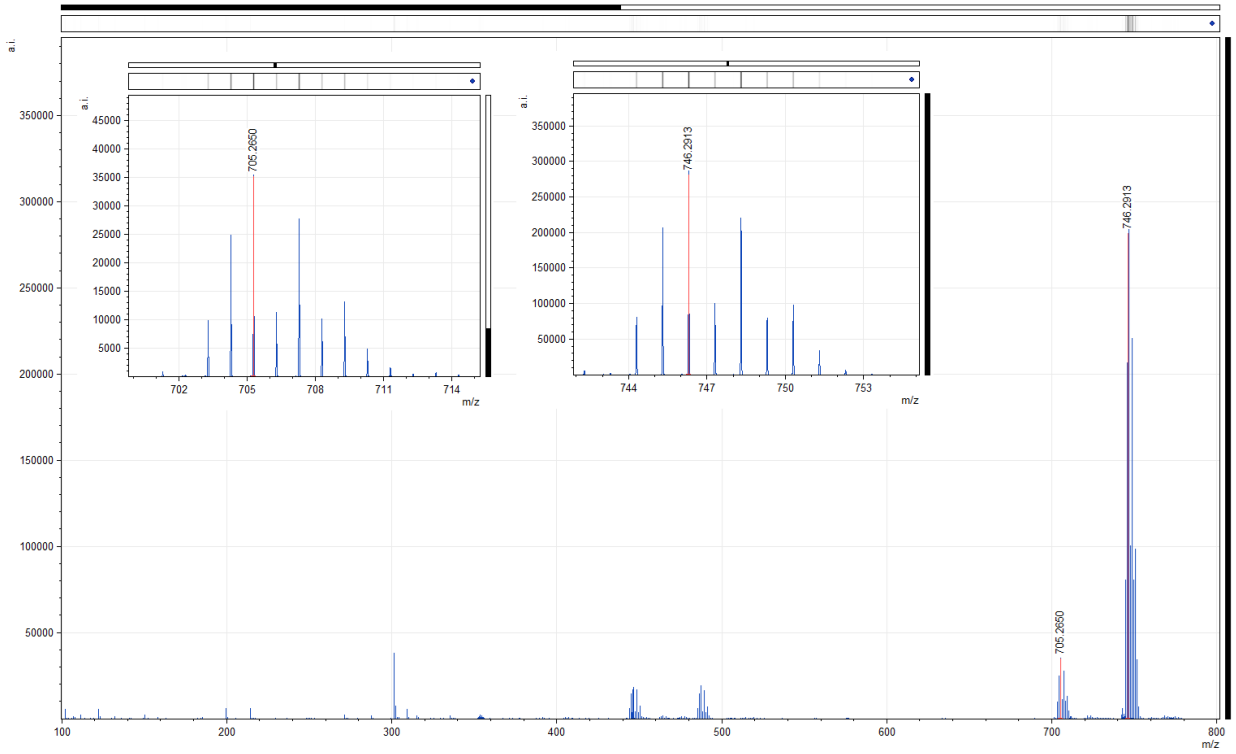


Spectrum S9. ^{1}H NMR spectrum of **ILe$_2$Ni** in DMSO-d_6.

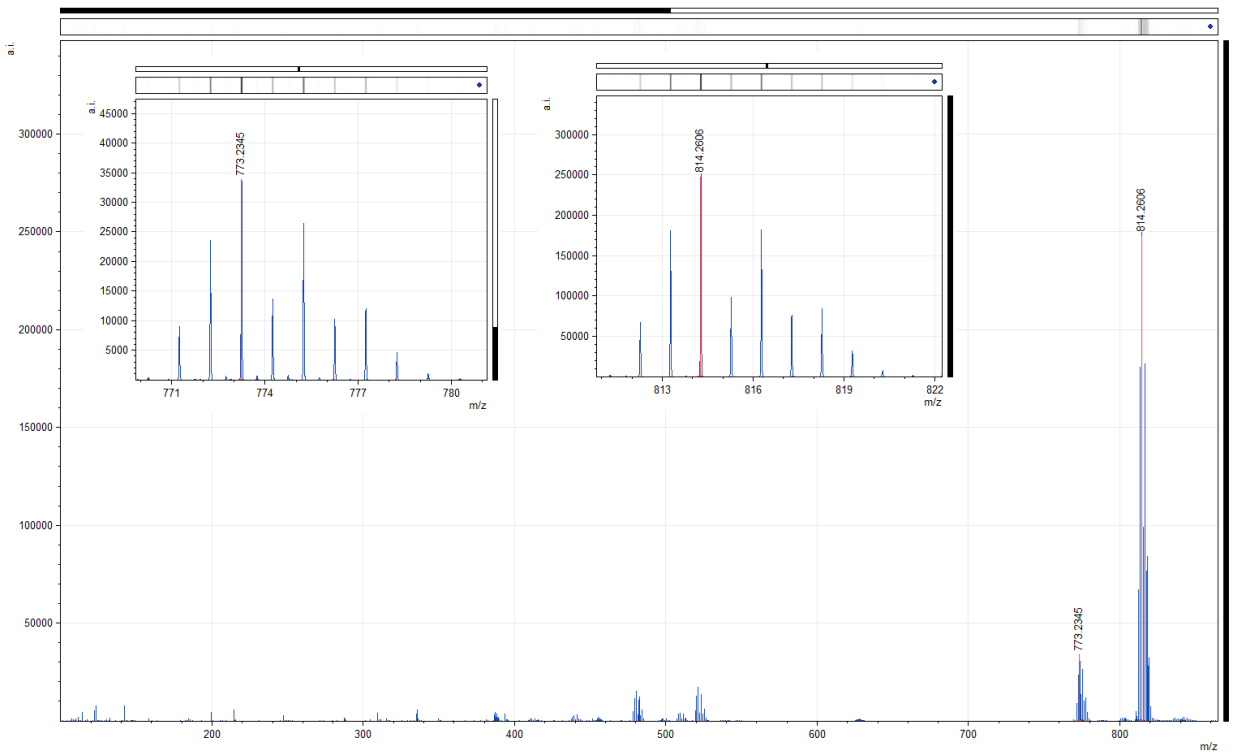


Spectrum S10. ^{1}H NMR spectrum of **Phe$_2$Ni** in DMSO-d_6.

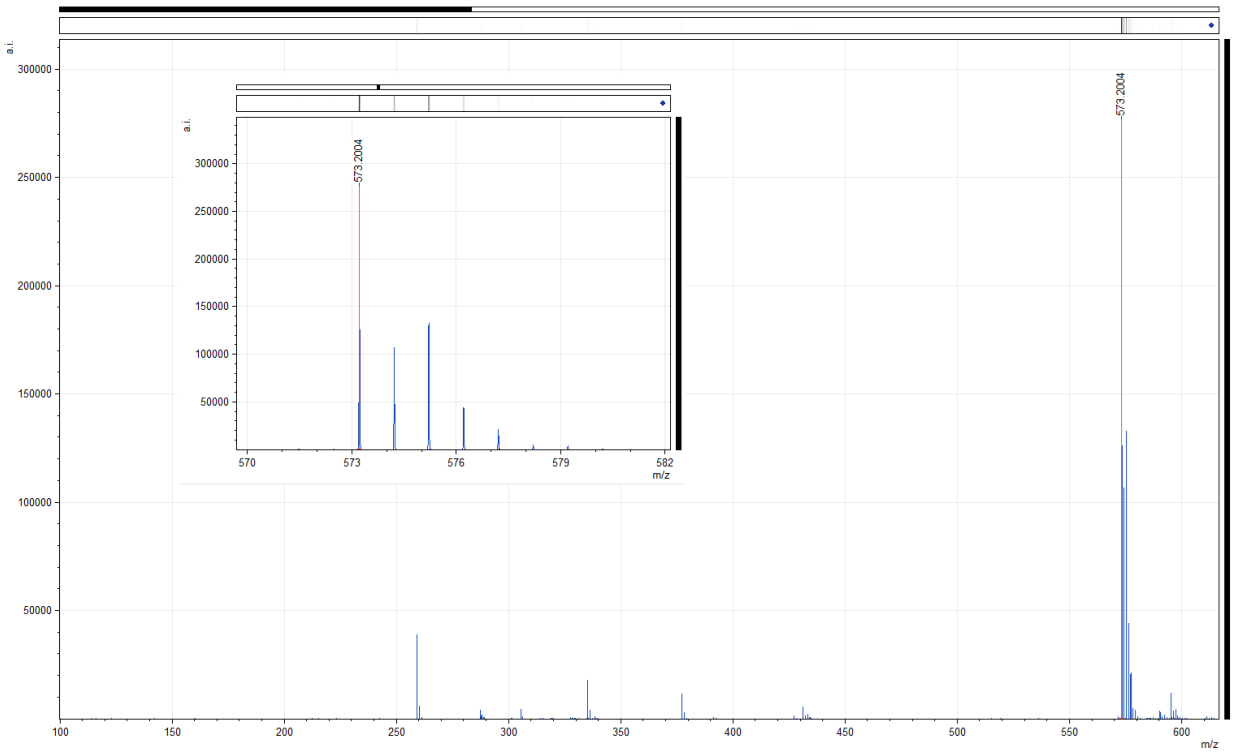
HR-MS spectra of metal complexes



Spectrum S11. HR-MS spectrum of I**Le$_2$Pd**. Insets: magnified view showing the isotopic distribution for $[M + H]^+$ (left) and $[M +MeCN + H]^+$ (right) ion peaks.



Spectrum S12. HR-MS spectrum of **Phe$_2$Pd**. Insets: magnified view showing the isotopic distribution for $[M + H]^+$ (left) and $[M +MeCN + H]^+$ (right) ion peaks.



Spectrum S13. HR-MS spectrum of **Ala_2Ni**. Inset: magnified view showing the isotopic distribution for $[M + H]^+$ ion peak.

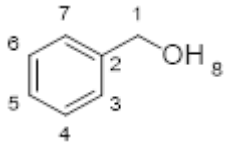
Catalysis: Procedure for the catalytic hydrosilylative reduction of aldehydes and ketones

To a schlenk under inert atmosphere it is added the catalyst **AA_2M** (**M** = Ni, Pd) (for aldehydes 7 mol%, 0.021 mmol; for ketones 10 mol%, 0.03 mmol), the solvent (0.2 M), the substrate (1 equiv, 0.3 mmol) and $PhSiH_3$ (1 equiv, 0.36 mmol, 46 µL). The reaction is stirred in an oil bath at the preset temperature for the preset time. The crude is treated with 5 mL of NaOH in MeOH (2 M) and stirred for 10 min. Et_2O (10 mL) and water (10 mL) are added, the phases separated, the aqueous one is extracted with additional Et_2O (2 x 10 mL), the combined organic phases dried over $MgSO_4$ and the volatiles evaporated under vacuum. The product is purified through chromatography in silica gel in a pipette using hex:AcOEt (9:1) as eluent.

Substrate conversion and identification of the catalytic products were determined by GC-MS analysis of the crude reaction mixture after the corresponding alcohol was formed by treatment with NaOH/MeOH. After the extraction and purification protocol, the isolated alcohols were identified by GC-MS again and then used for further characterization by NMR in the case of aldehyde derivatives, whereas those derived from ketones were used to analyse possible enantiomeric excesses (ee) by HPLC (Agilent HPLC Series 1200 with UV-Vis detector and Chiralcel OD-H column). Unfortunately, no ee was observed with any of the ketones tested.

Substrate scope: aldehydes

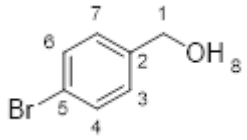
Benzyl alcohol (2a).[3]



Synthetized from benzaldehyde (**1a**).

^{1}H NMR (300 MHz. DMSO-d_6) δ = δ 7.43 – 7.17 (m; 5H; 3-7); 5.18 (t; *J* = 5.5; 1H; 8); 4.50 (d; *J* = 5.6; 2H; 1). CG-MS, retention time: for C_7H_8O m/z = 108.06, t = 10.0 min.

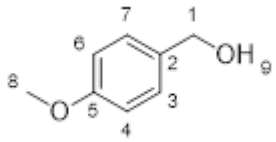
(4-bromophenyl)methanol (2b).[3]



Synthetized from 4-bromobenzaldehyde (**1b**).

^{1}H NMR (400 MHz. DMSO-d_6) δ = 7.49 (d; *J* = 8.3; 2H; 4, 6); 7.26 (d; *J* = 8.3; 2H; 3, 7); 5.25 (td; *J* = 5.7, 0.9; 1H; 8); 4.44 (d; *J* = 5.7; 2H; 1). CG-MS, retention time: for C_7H_7OBr m/z = 185.97, t = 18.4 min.

(4-methoxyphenyl)methanol (2c).[3]



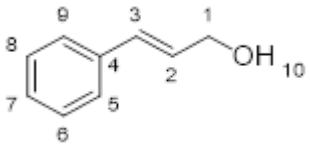
Synthetized from 4-methoxybenzaldehyde (**1c**).

^{1}H NMR (400 MHz. DMSO-d_6) δ = 7.49 (d; *J* = 8.3; 2H; 4, 6); 7.26 (d; *J* = 8.3; 2H; 3, 7); 5.25 (td; *J* = 5.7, 0.9; 1H; 8); 4.44 (d; *J* = 5.7; 2H; 1). CG-MS, retention time: for $C_8H_{10}O_2$ m/z = 138.07, t = 17.1 min.

---

[3] L. Shi, Y. Liu, Q. Liu, B. Wei, G. Zhang *Green Chem.* **2012**,*14*, 1372-1375.

3-phenylprop-2-en-1-ol (2d).[3]

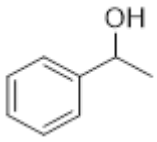


Synthetized from cinnamaldehyde (**1d**).

^{1}H NMR (400 MHz. $CDCl_3$) δ = 7.42 (dd; *J* = 8.3 and 1.3; 2H; 5, 9); 7.32 (t; *J* = 7.4; 2H; 6, 8); 7.27 – 7.16 (m; 1H; 7); 6.56 (dt; *J* = 15.9, 1.7; 1H; 3); 6.38 (dt; *J* = 15.9, 5.0; 1H; 2); 4.88 (t; *J* = 5.4; 1H; 10); 4.13 (td; *J* = 5.2, 1.7; 2H; 1). CG-MS, retention time: for $C_9H_{10}O$ m/z = 134.07, t = 17.5 min.

Substrate scope: ketones

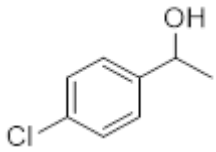
1-phenylethan-1-ol (4a).



Synthetized from acetophenone (**3a**).

CG-MS, retention time: for $C_8H_{10}O$ m/z = 122.07, t = 10.8 min.

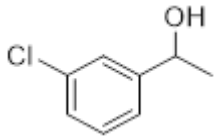
1-(4-chlorophenyl)ethan-1-ol (4b).



Synthetized from 4-chloroacetophenone (**3b**).

CG-MS, retention time: for C_8H_9OCl m/z = 156.03, t = 16.6 min.

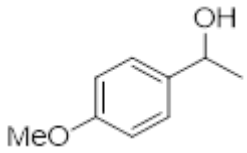
1-(3-chlorophenyl)ethan-1-ol (4c).



Synthetized from 3-chloroacetophenone (**3c**).

CG-MS, retention time: for C_8H_9OCl m/z = 156.03, t = 18.8 min.

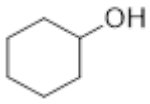
1-(4-methoxyphenyl)ethan-1-ol (4e).



Synthetized from 4-methoxyacetophenone (**3e**).

CG-MS, retention time: for $C_9H_{12}O_2$ m/z = 152.08, t = 17.6 min.

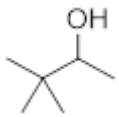
Cyclohexanol (4f)



Synthetized from cyclohexanone (**3f**).

CG-MS, retention time: for $C_6H_{12}O$ m/z = 100.09, t = 5.8 min

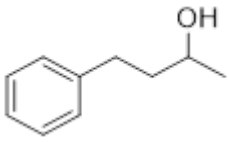
3,3-dimethylbutan-2-ol (4g)



Synthetized from tertbutylmethylketone (**3g**).

CG-MS, retention time: for $C_6H_{14}O$ m/z = 102.10, t = 2.8 min.

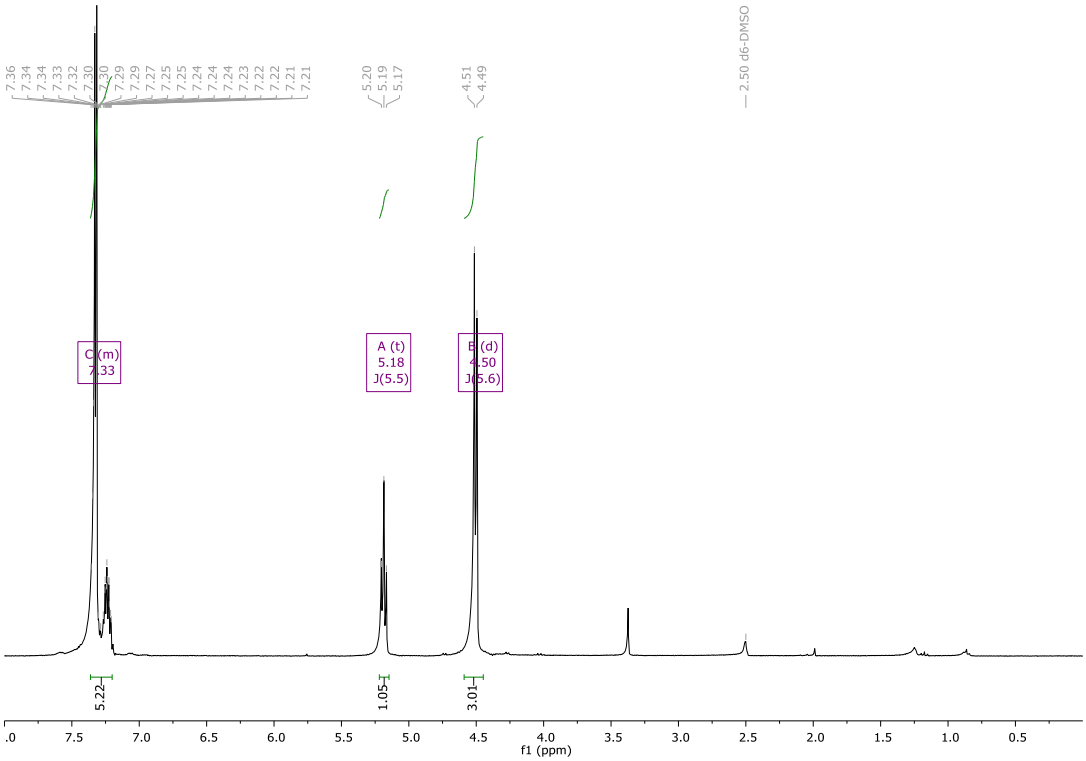
4-phenylbutan-2-ol (7h)



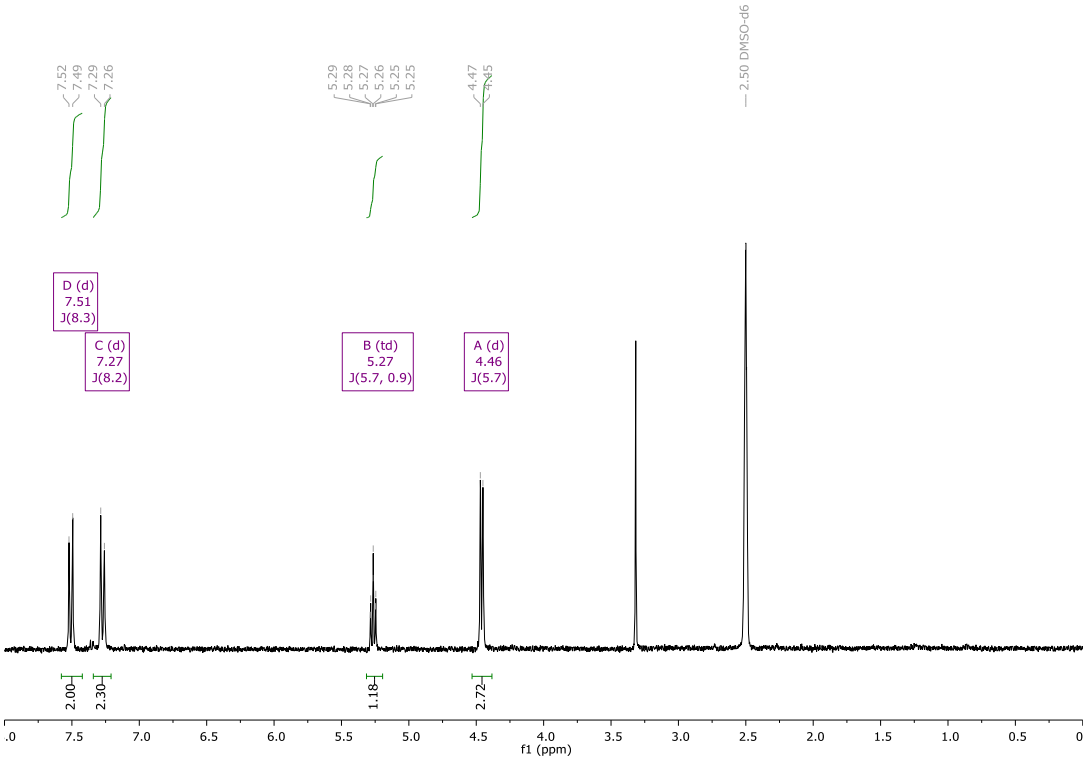
Synthetized from 4-phenylbut-3-en-2-one (**3h**).

CG-MS, retention time: for $C_{10}H_{14}O$ m/z = 150.10, t = 18.6 min.

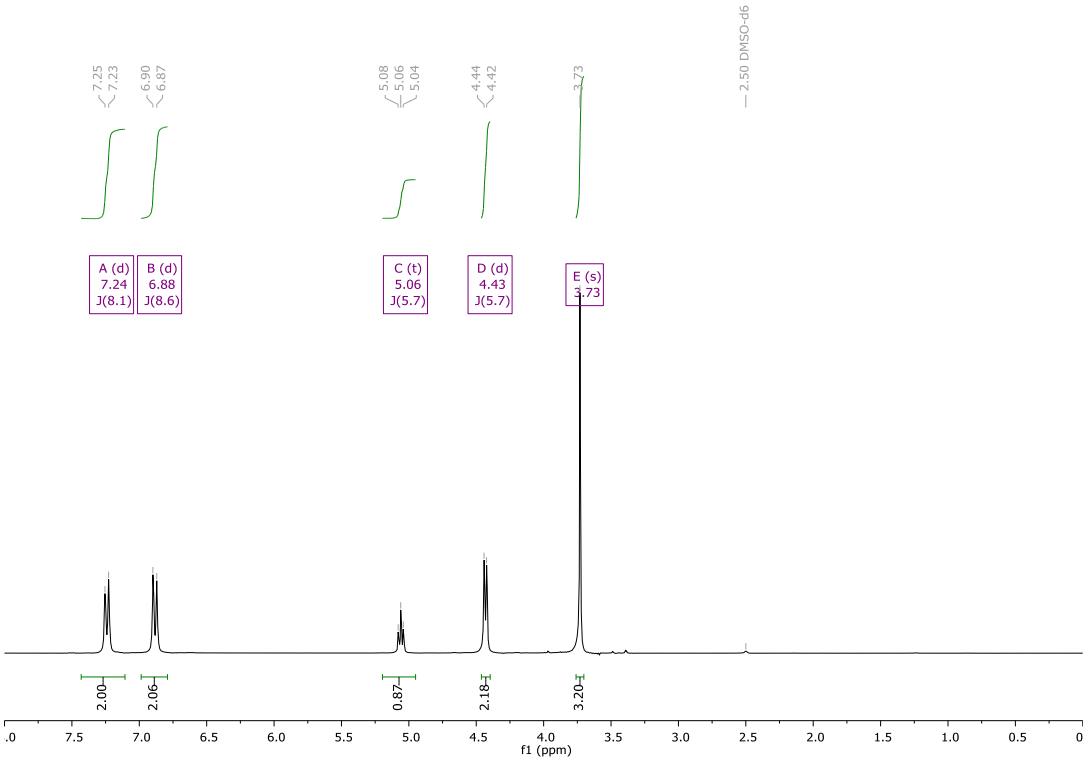
^{1}H NMR spectra of alcohols obtained by reducing aldehydes



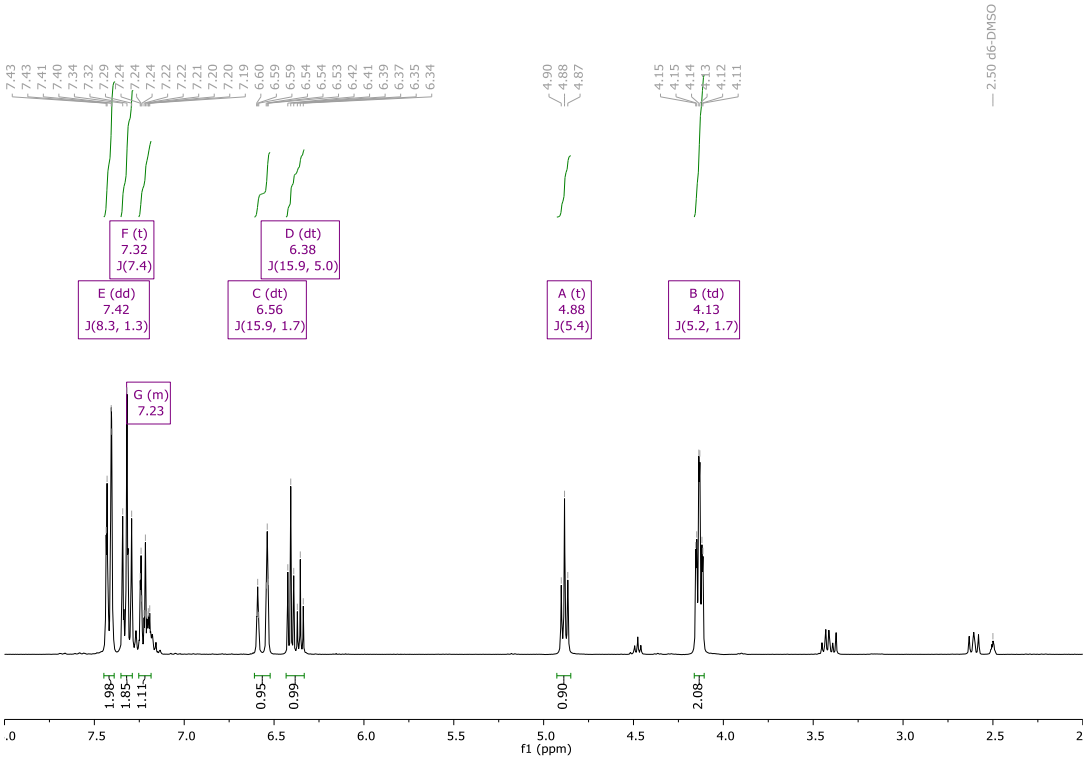
Spectrum S14. ^{1}H NMR spectrum of benzyl alcohol (**2a**) obtained from benzaldehyde in DMSO-d_6.



Spectrum S15. ^{1}H NMR spectrum of (4-bromophenyl)methanol (**2b**) obtained from 4-bromobenzaldehyde in DMSO-d_6.

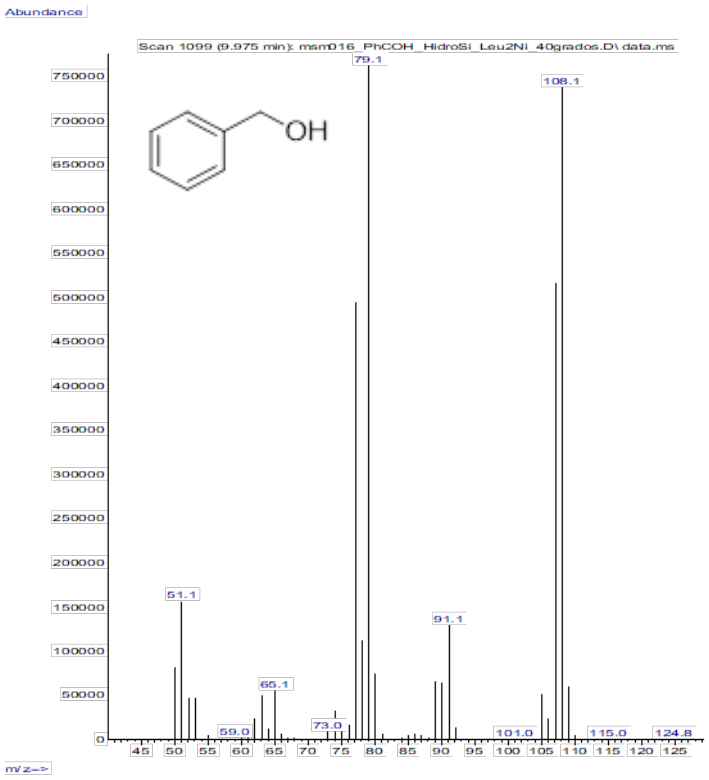


Spectrum S16. ^{1}H NMR spectrum of (4-methoxyphenyl)methanol (**2c**) obtained from 4-methoxybenzaldehyde in DMSO-d_6.

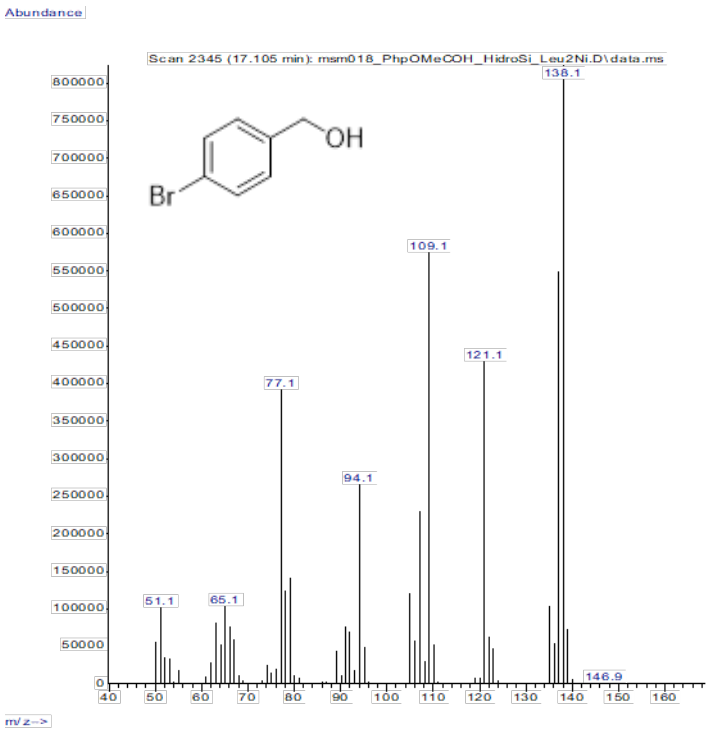


Spectrum S17. ^{1}H NMR spectrum of 3-phenylprop-2-en-1-ol (**2d**) obtained from cinnamaldehyde in $CDCl_3$.

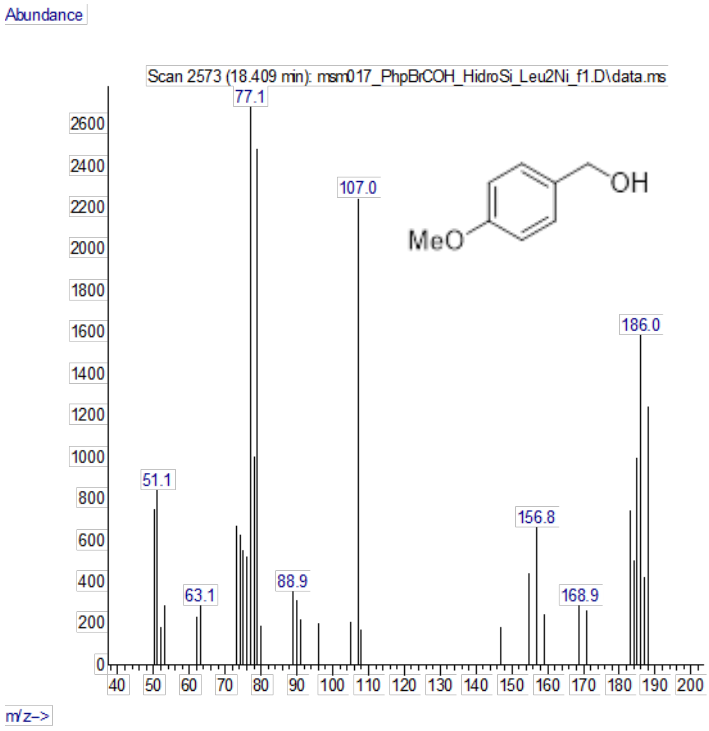
GC-MS spectra of alcohols obtained by reducing aldehydes and ketones



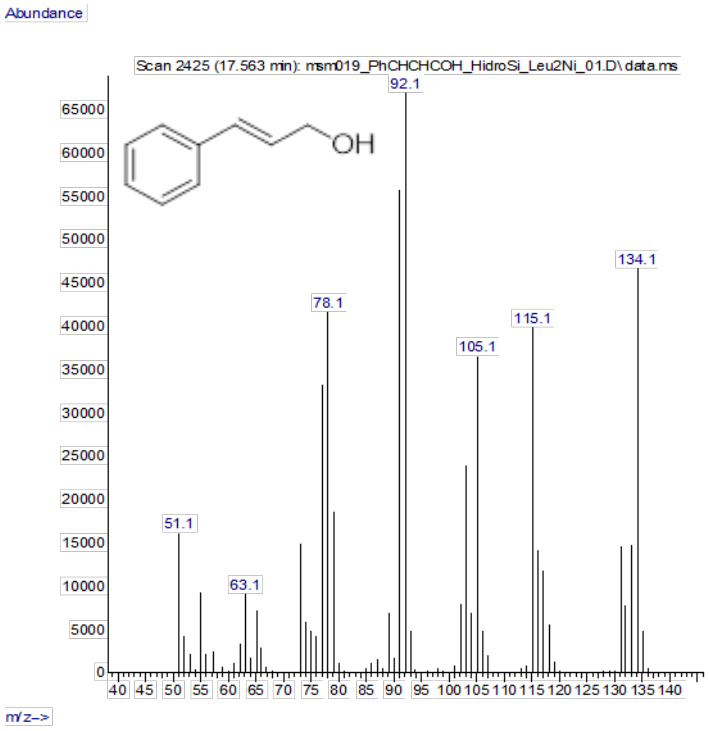
Spectrum S18. Mass spectrum of benzyl alcohol (**2a**) obtained from benzaldehyde.



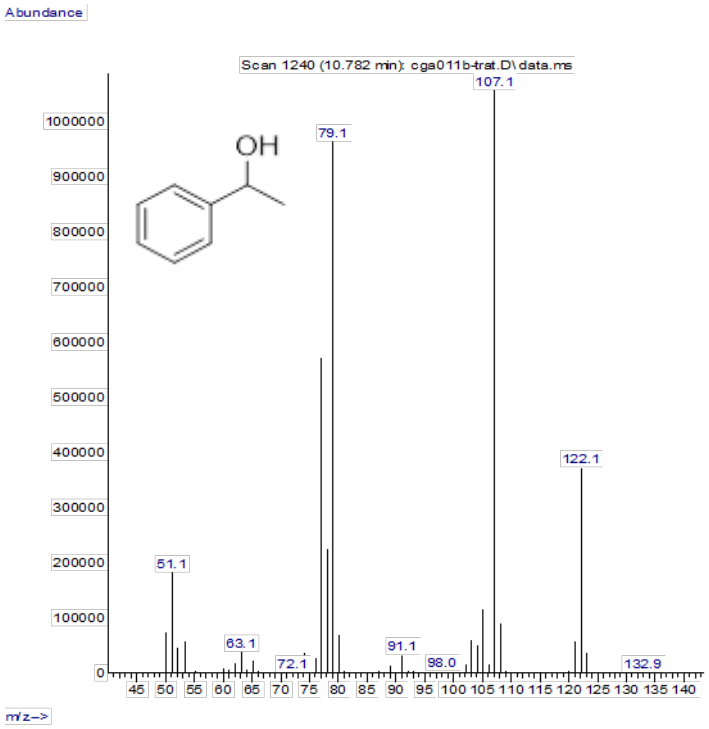
Spectrum S19. Mass spectrum of (4-bromophenyl)methanol (**2b**) obtained from 4-bromobenzaldehyde.



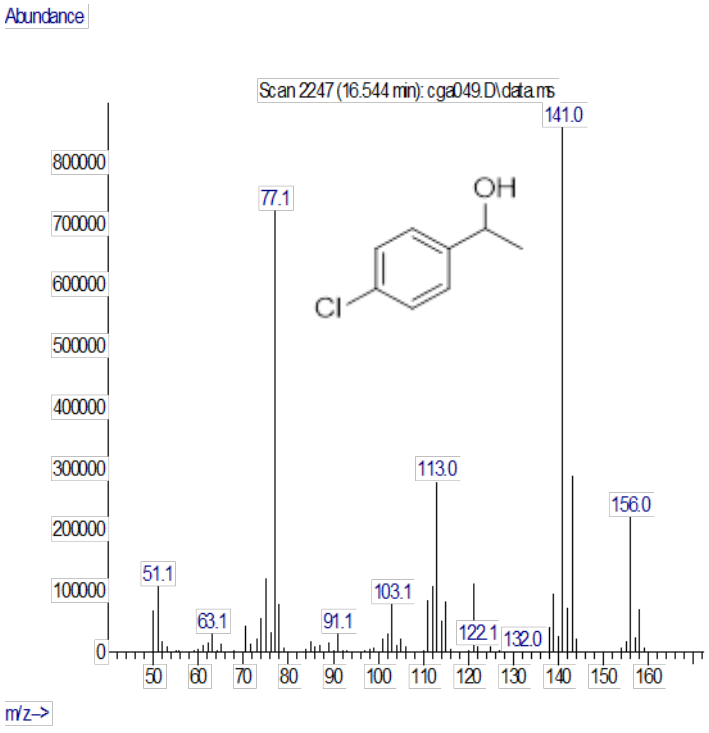
Spectrum S20. Mass spectrum of (4-methoxyphenyl)methanol (**2c**) obtained from 4-methoxybenzaldehyde.



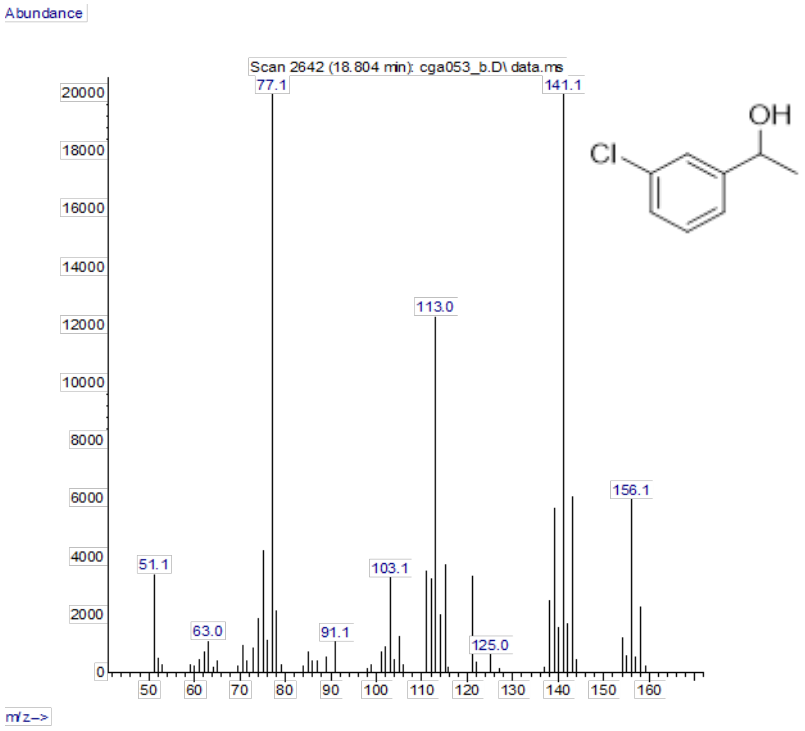
Spectrum S21. Mass spectrum of 3-phenylprop-2-en-1-ol (**2d**) obtained from cinnamaldehyde.



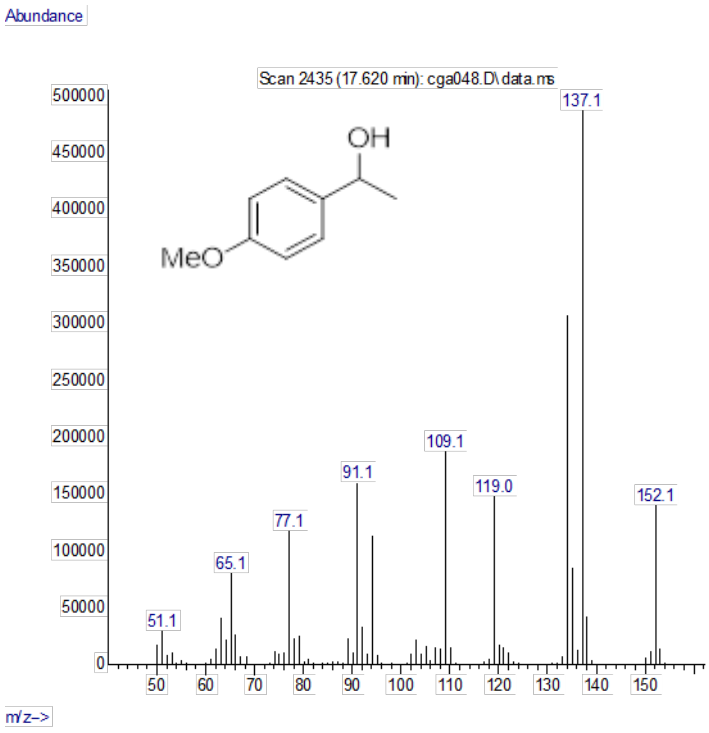
Spectrum S22. Mass spectrum of 1-phenylethan-1-ol (**4a**) obtained from acetophenone.



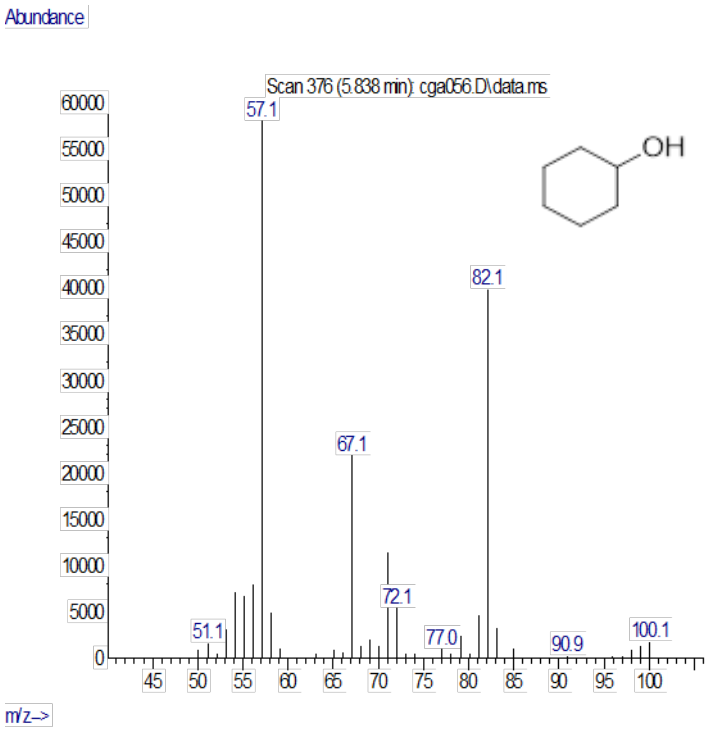
Spectrum S23. Mass spectrum of 1-(4-chlorophenyl)ethan-1-ol (**4b**) obtained from 4-chloroacetophenone.



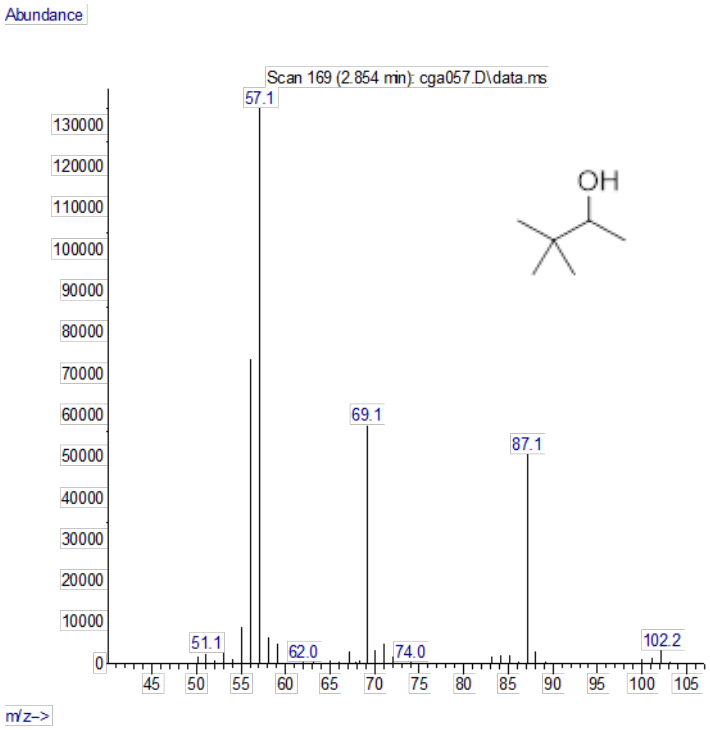
Spectrum S24. Mass spectrum of 1-(3-chlorophenyl)ethan-1-ol (**4c**) obtained from 3-chloroacetophenone.



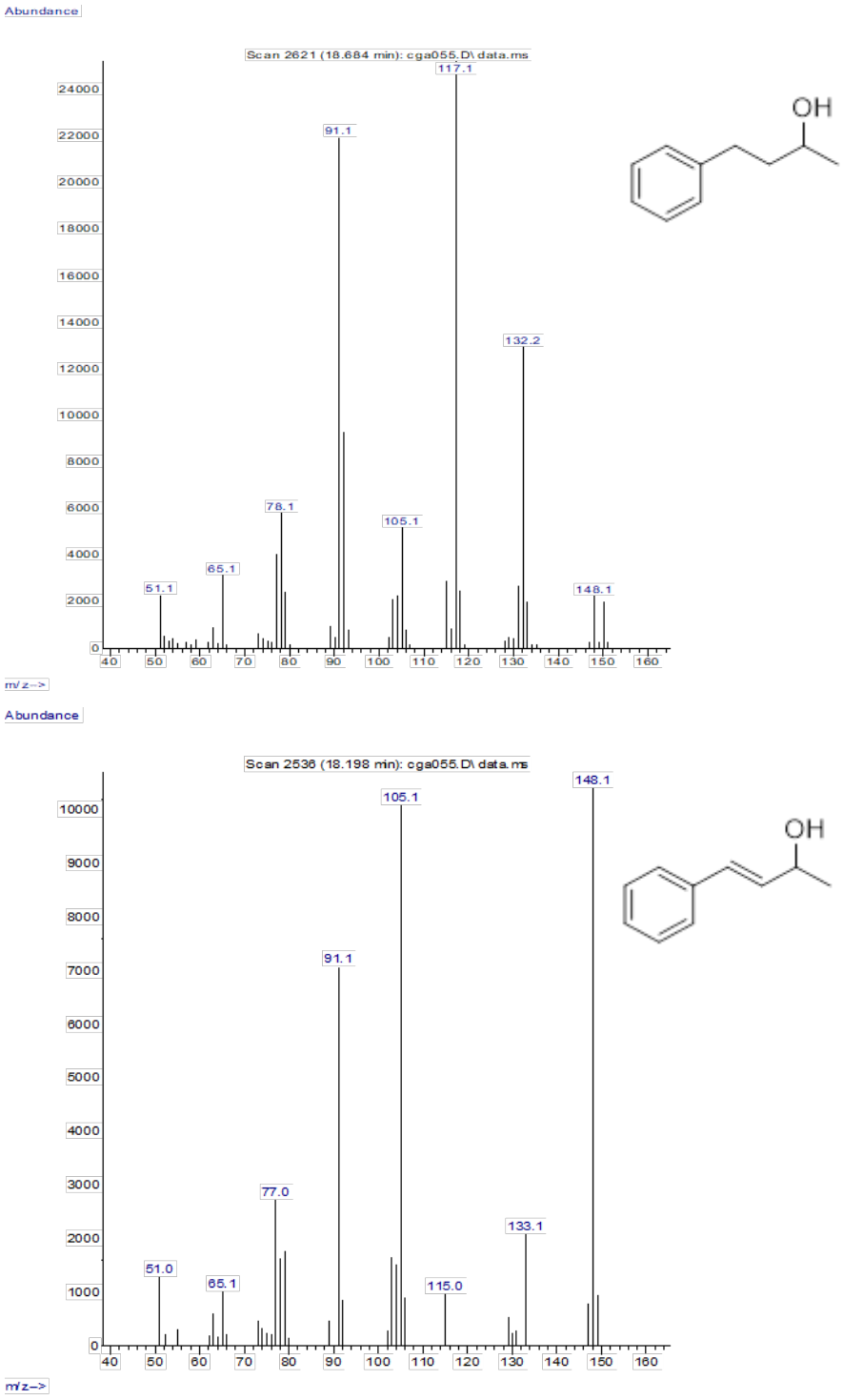
Spectrum S25. Mass spectrum of 1-(4-methoxyphenyl)ethan-1-ol (**4e**) obtained from 4-methoxyacetophenone.



Spectrum S26. Mass spectrum of cyclohexanol (**4f**) obtained from cyclohexanone.



Spectrum S27. Mass spectrum of 3,3-dimethylbutan-2-ol (**4g**) obtained from tertbutylmethylketone.



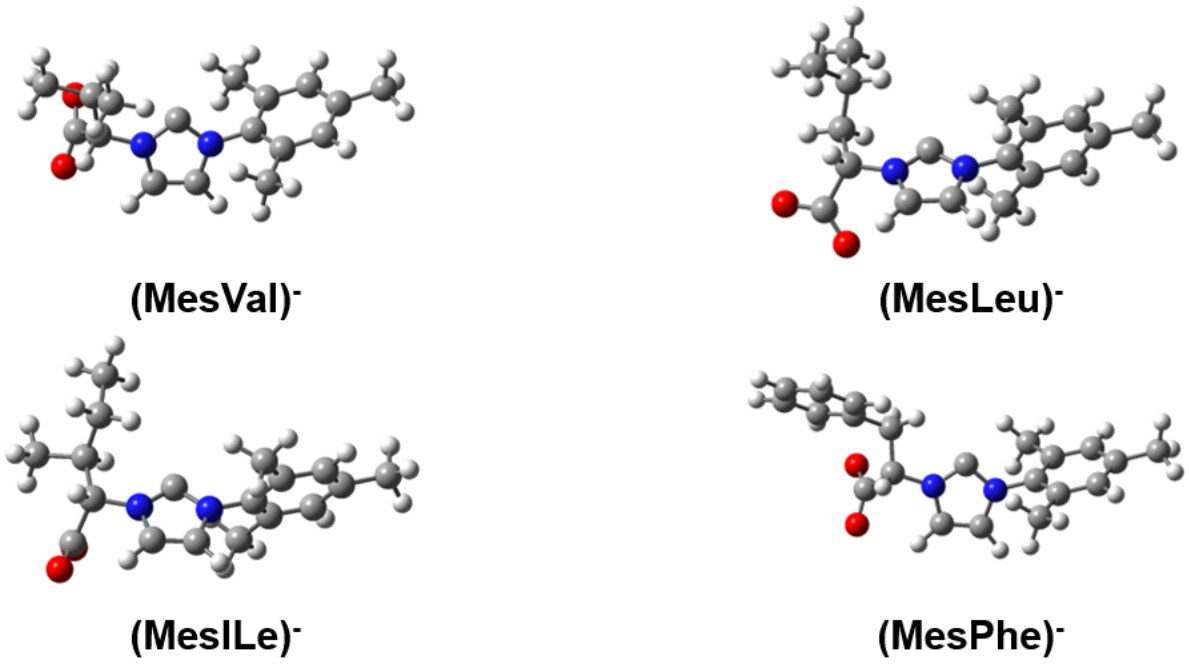
Spectrum S28. Mass spectrum of 4-phenylbutan-2-ol (**7h**, up) and semi-reduced 4-phenylbut-3-en-2-ol (**5h**, down) obtained from 4-phenylbut-3-en-2-one.

Theoretical results

Computational Details

The electronic structure and geometries of the (**MesAA**)$^-$ ligands, **AA$_2$Ni** complexes and species of the reaction between PhCHO and $PhSiH_3$ were investigated using density functional theory at the mpw1pw91 level[4] with the 6-311+G(d,p) basis set. Single-point calculations on the fixed conformation of (**MesAA**)$^-$ ligands in **AA$_2$Ni** complexes were used to obtain the molecular orbitals of coordinated ligands. For the calculation of the TEP parameter of (**MesAA**)$^-$ ligands, a modification of the approach used by Gusev was adopted,[5] with the description of the Ni atom using the 6-311+G(2d) basis set. Frequency calculations were carried out at the same theoretical level to identify all the stationary points as minima (zero imaginary frequencies) and to provide the thermal correction to free energies at 298.15 K and 1 atm. Molecular geometries were optimized without symmetry restrictions. DFT calculations were performed using the Gaussian 09 suite of programs.[6] The coordinates of optimized compounds are reported in Table S5.

Figure S2. Optimized structures of (**MesAA**)$^-$ ligands.



[4] C. Adamo, V. Barone, *J. Chem. Phys.* **1998**, *108*, 664–675.
[5] D. G. Gusev, *Organometallics* **2009**, *28*, 6458–6461.
[6] Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

Figure S3. HOMO-3 of the free (**MesAA**)$^-$ ligands.

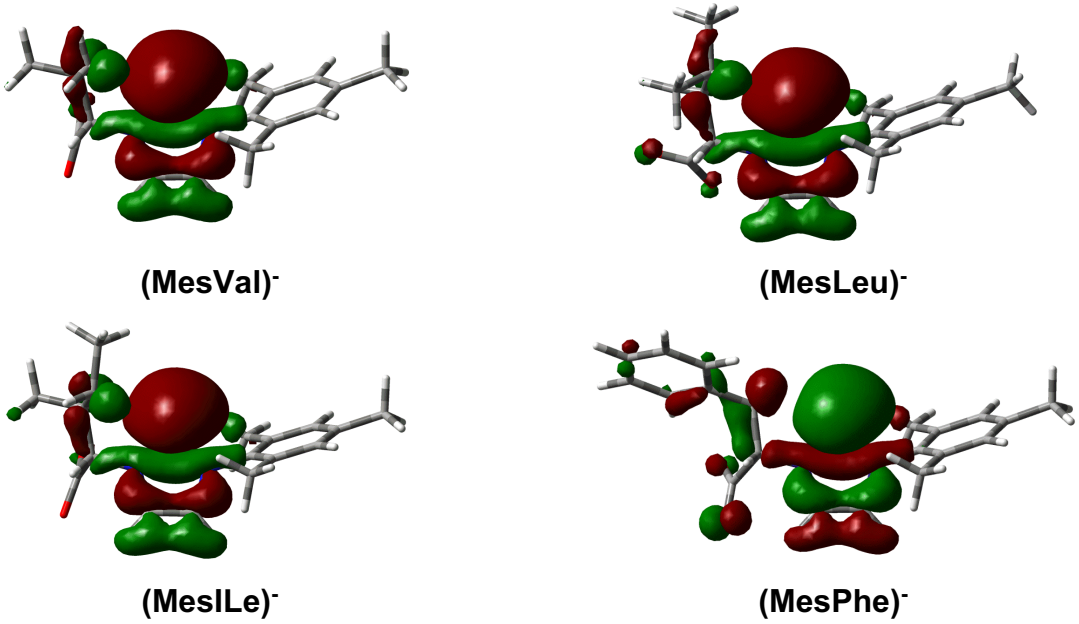
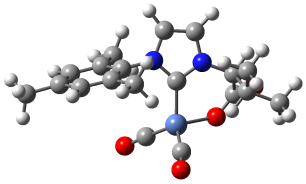
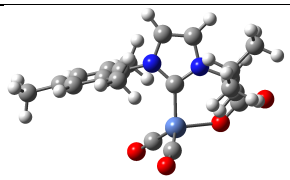
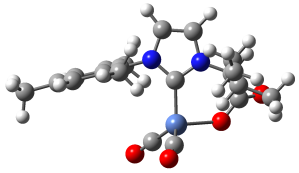
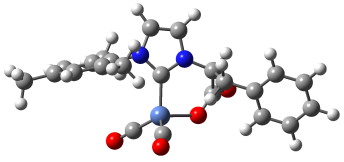


Table S1. Optimized structures of complexes [Ni(CO)$_2$(κ^2-**AA**)]$^-$ and their calculated properties.[a]

AA	TEP (cm^{-1}) [b]	Unscaled ν_{CO} (A_1)	d(Ni-C) (Å)	d(Ni-O) (Å)	Optimized structures
Val	1955.8	2049.9	1.943	2.145	
Leu	1955.2	2049.3	1.941	2.139	
ILe	1955.9	2050.0	1.943	2.147	
Phe	1959.8	2054.0	1.944	2.160	

[a] The mPW1PW91 functional and the basis sets 6-311+G(2d) for Ni and 6-311+G(d,p) for all other atoms were used for the calculations. Optimizations were carried out without symmetry restrictions, with the tight option and the ultrafine integration grid. [b] Scaled carbonyl stretching frequencies by a factor of 0.9541.

Table S2. Percent buried volume, $\%V_{bur}$, of (**MesAA**)$^-$ ligands, calculated from the X-ray data of **AANiCp** complexes.[a]

AA	$\%V_{bur}$
	AANiCp
Val	45.0
Leu	45.2
ILe	45.2
Phe	46.7

[a] Data from reference 2.

Table S3. Comparison of selected experimental and calculated structural parameters for complex **Leu_2Ni**.

	Experimental	**Calculated**
	X-ray	**DFT (mpw1pw91/6-311+G(d,p))**
Ni-C	1.900(3)	1.919
	1.915(3)	1.922
Ni-O	1.858(3)	1.863
	1.852(3)	1.865
C-Ni-C	176.9(1)	178.5
O-Ni-O	177.3(1)	178.5
O-Ni-C	90.5(1)	91.5
	91.3(1)	91.6

Figure S4. Correlation between the calculated TEP values for the (**MesAA**)$^-$ ligands and the energies of the HOMO (up) and HOMO–3 (bottom).

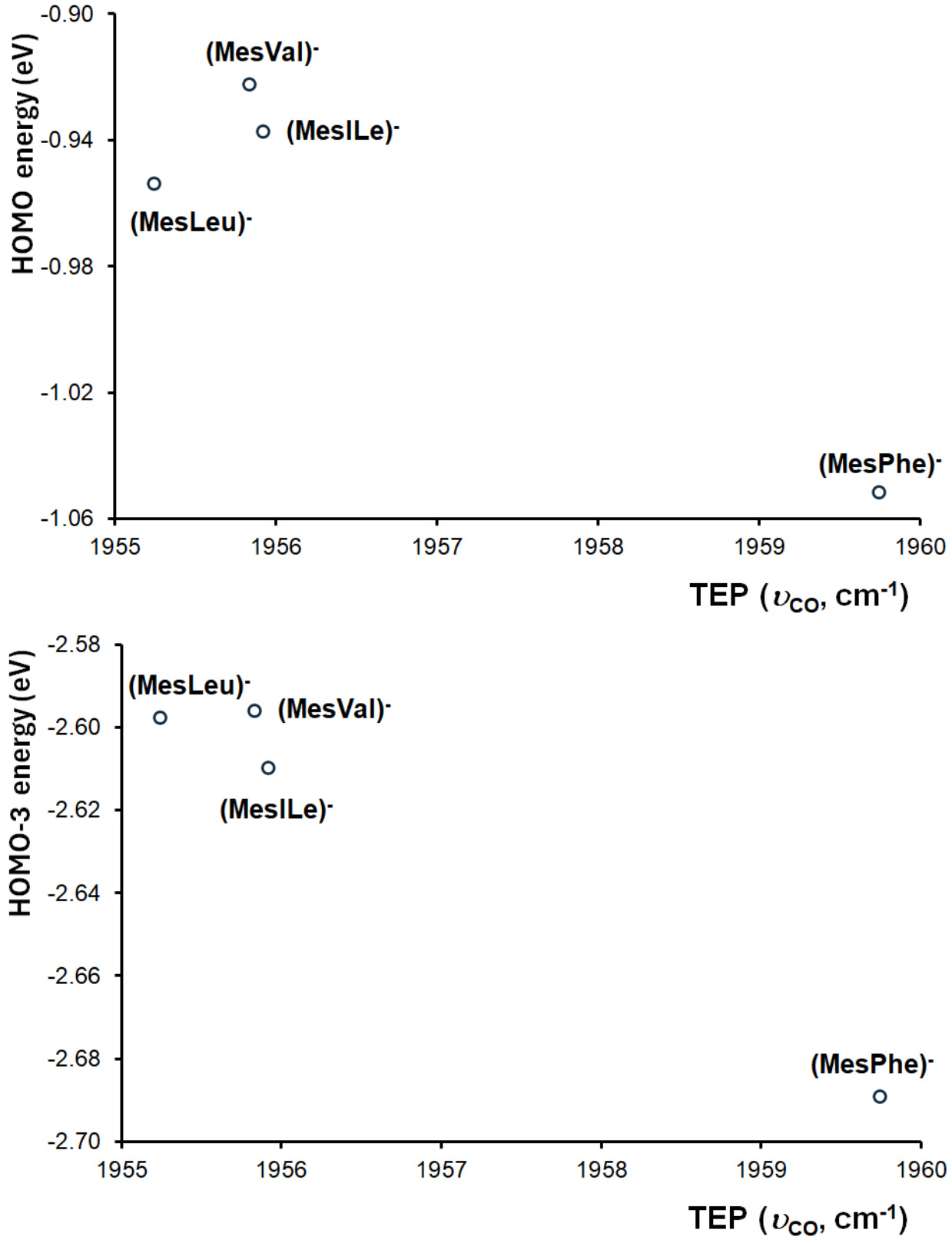


Figure S5. Optimized structures of complex **Leu$_2$Ni** (up), complex **Leu$_2$Ni** with a dissociated carboxylate arm (middle) and a conformer of **Leu$_2$Ni** (bottom). Hydrogen atoms are omitted for clarity.

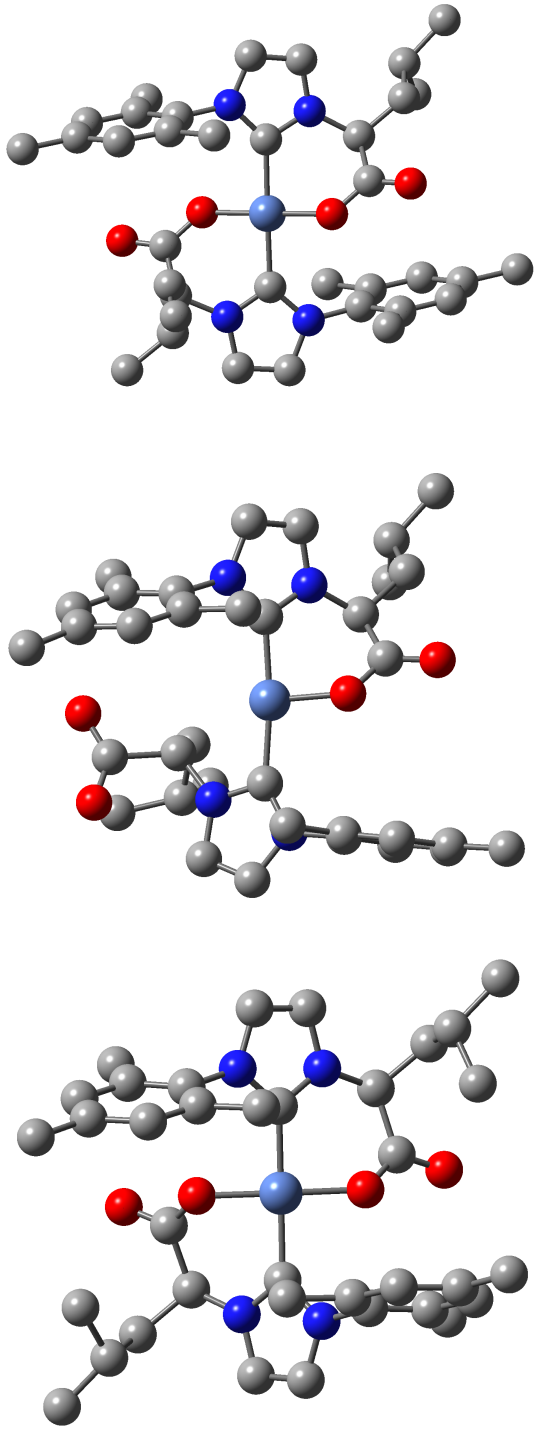


Figure S6. Relative energy profile for the non-catalysed reaction between PhCHO and $PhSiH_3$ (gas phase).

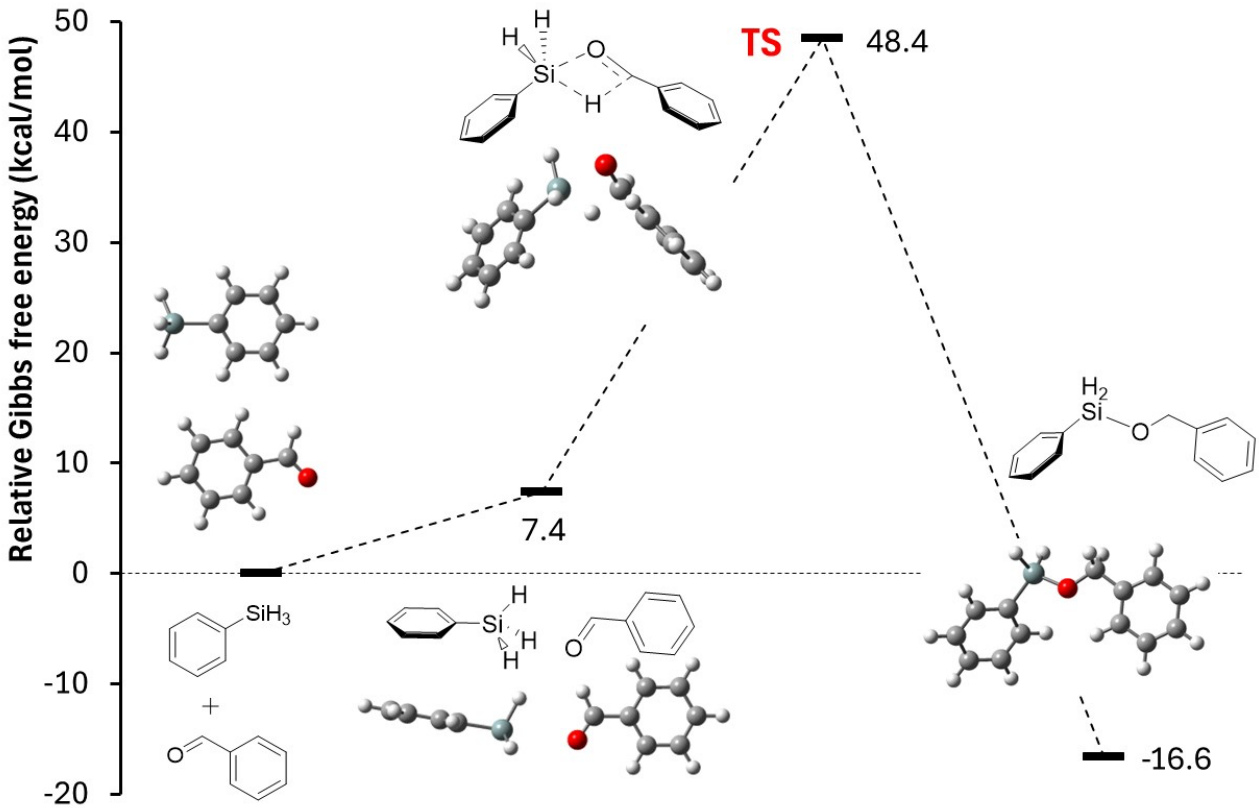
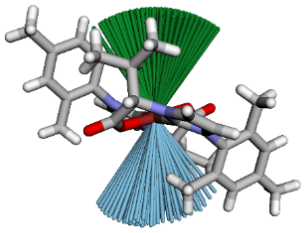
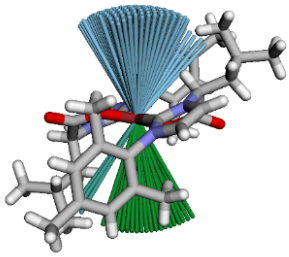
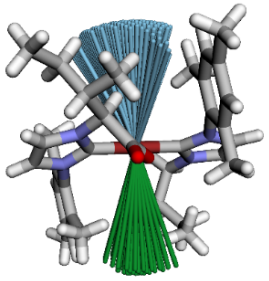


Table S4. Application of *AtomAcces* to **AA_2Ni** complexes.[a]

AA	Val	Leu	Ile
***AtomAcces* output**			
% unblocked	7.6	9.7	7.1

[a] *AtomAccess*: https://www.nfchilton.com/atom_access (accessed 2025-12-4). This tool calculates the sizes of accessible coordination sites in a complex, and it is expressed as a solid angle percentage.

Figure S7. Structural comparison of the two conformers of complex **Leu$_2$Ni** (Mes groups are omitted for clarity).

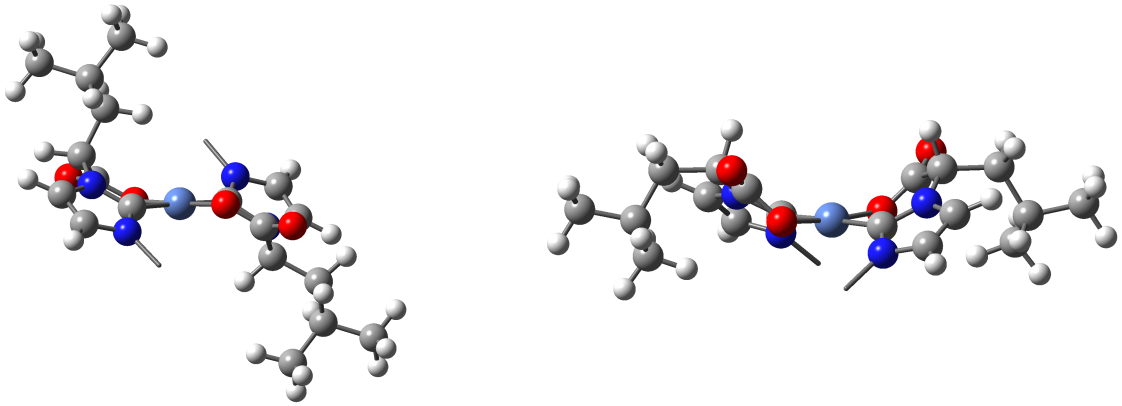


Table S5. Coordinates of the optimized compounds.

Ligands (MesAA)$^-$.

Val

O	-3.64804600	-1.94033400	-0.37321700
O	-4.06047900	-1.11359000	1.68795500
N	-1.58661200	0.25435900	0.54858500
N	0.52594400	0.07603800	0.63309100
C	-0.49824400	0.25853400	-0.26038000
C	-1.26667200	0.05931300	1.88079100
H	-2.03792200	-0.04781200	2.62565800
C	0.07769100	-0.04968200	1.94425200
H	0.73753000	-0.22752100	2.77676700
C	1.88929700	-0.01096600	0.24236300
C	2.75425700	1.05299600	0.51047800
C	4.09216400	0.93476100	0.13527500
H	4.76789700	1.76095100	0.33810200
C	4.57523600	-0.20223000	-0.50335700
C	3.68398100	-1.24055700	-0.76420400
H	4.04174400	-2.13690600	-1.26303800
C	2.34117500	-1.16884100	-0.40284600
C	2.24889900	2.30751300	1.16239900
H	1.32430500	2.64168200	0.68727900
H	2.99123400	3.10462500	1.09107100
H	2.01958400	2.15115300	2.21996400
C	6.01252300	-0.29661000	-0.93550300
H	6.12145000	-0.05280100	-1.99741900
H	6.40625900	-1.30581200	-0.79228000
H	6.64327200	0.39520600	-0.37335300
C	1.39783500	-2.29610600	-0.69772900
H	0.90612500	-2.64956200	0.21187200
H	1.92593300	-3.13315100	-1.15789600
H	0.59789500	-1.96288200	-1.36231300
C	-2.99800500	0.32333800	0.12619000
H	-3.47025700	1.07585200	0.76798300
C	-3.65057000	-1.06616100	0.50818100
C	-3.16568500	0.74393700	-1.33026400
H	-2.60634500	0.02995100	-1.94043300
C	-4.64229600	0.66224800	-1.71682900
H	-5.01120500	-0.35726100	-1.60694300
H	-4.78026500	0.97802600	-2.75625500
H	-5.24957600	1.32426800	-1.08776400
C	-2.63614800	2.15369300	-1.59383400
H	-3.16204600	2.88808800	-0.97159500
H	-2.79822300	2.43369300	-2.64054600
H	-1.56715400	2.21773700	-1.38839800

Leu

O	-2.97101400	-2.76857700	-0.10372000
O	-4.81360800	-1.50961100	-0.43770100
N	-1.42832900	-0.59982400	0.52442100
N	0.69509700	-0.56214500	0.53372100
C	-0.38196300	0.01190300	-0.08688800
C	-1.02706200	-1.52060400	1.47178300
H	-1.72941300	-2.14609500	1.99244700
C	0.32291400	-1.49722900	1.49549900
H	1.03471100	-2.07241600	2.06344900
C	2.04189100	-0.24781800	0.20770200
C	2.77810300	0.58991900	1.04970400
C	4.10273500	0.87003300	0.71801200
H	4.67694600	1.52784400	1.36446900
C	4.69774600	0.34475800	-0.42478300
C	3.93057300	-0.47198000	-1.25162300
H	4.37289400	-0.88059900	-2.15583200
C	2.60502000	-0.78200000	-0.95649200
C	2.14127300	1.20212500	2.26317000
H	1.19669900	1.68191200	1.99747600
H	2.80175500	1.94552200	2.71317900
H	1.90712100	0.44888100	3.01991100
C	6.13746200	0.63347600	-0.74913500
H	6.46682100	1.57083100	-0.29570700
H	6.29595700	0.70555600	-1.82756800
H	6.79326300	-0.16005900	-0.37545600
C	1.78927300	-1.64969000	-1.86728000
H	1.34564300	-2.48822400	-1.32557200
H	2.40110400	-2.04059900	-2.68230300
H	0.95365400	-1.08311200	-2.28415300
C	-2.84933100	-0.37609800	0.22910200
H	-3.31655400	-0.06630700	1.17095500
C	-3.61653400	-1.70825500	-0.16146000
C	-3.05587300	0.71296900	-0.81256000
H	-2.41236800	0.49073800	-1.66863700
H	-4.09413400	0.60728600	-1.14007700
C	-2.79856600	2.15614300	-0.36352500
H	-1.79667500	2.19539500	0.07721700
C	-2.80527000	3.08286000	-1.57690300
H	-2.03119300	2.79043700	-2.29134500
H	-2.62480500	4.12454900	-1.29012100
H	-3.77137100	3.04131400	-2.09309300
C	-3.81489400	2.63197700	0.67224400
H	-4.82993200	2.60615600	0.26099400
H	-3.60495400	3.65987800	0.98736100
H	-3.81054100	2.00545100	1.56738400

lLe

O	-3.42540300	-1.66002400	-1.43390800
O	-3.86364400	-2.32004400	0.68159800
C	-3.46334700	-1.52979400	-0.19986500
C	-2.87072500	-0.18427700	0.38345300
H	-3.33754500	-0.03666700	1.36395100
C	-3.10161200	1.05868700	-0.47057000
H	-2.50596700	0.93977200	-1.38021300
C	-2.65745500	2.33840200	0.25341600
H	-1.69962300	2.15620700	0.74491900
H	-3.38762800	2.56945100	1.04126300
C	-2.49427700	3.54120800	-0.66907700
H	-1.72481900	3.33794900	-1.41909700
H	-2.18873700	4.43274900	-0.11184100
H	-3.42014900	3.78672200	-1.19729300
C	-4.57836900	1.14058800	-0.85872500
H	-4.85915800	0.27511600	-1.45814000
H	-4.78342900	2.04610400	-1.43706800
H	-5.21422700	1.16633100	0.03432100
C	-0.38951400	0.15075100	0.02059200
C	-1.05707000	-1.43373200	1.52365800
H	-1.79068400	-2.03922100	2.03020100
C	0.29183100	-1.48425000	1.48663500
H	0.99303200	-2.12437400	1.99525100
C	2.02548200	-0.25263900	0.19953100
C	2.86380800	0.43401800	1.08141800
C	4.18716900	0.65867700	0.70371400
H	4.84213100	1.19540300	1.38435900
C	4.68092000	0.22858200	-0.52328400
C	3.81583200	-0.44487400	-1.38255300

H	4.18237100	-0.78828800	-2.34585000
C	2.48835400	-0.69627600	-1.04533000
C	2.34381700	0.94366500	2.39441100
H	2.15676800	0.12986000	3.10019600
H	1.39322400	1.46271000	2.25536600
H	3.05822500	1.63103200	2.85115900
C	6.10013400	0.51435900	-0.93019500
H	6.52921900	-0.31912400	-1.49151500
H	6.73424200	0.69826600	-0.06036700
H	6.15524100	1.40063700	-1.57088200
C	1.57245100	-1.41835000	-1.98732800
H	0.73224400	-0.78058100	-2.26998200
H	1.13474200	-2.30153400	-1.51566800
H	2.10799900	-1.73064400	-2.88560500
N	-1.44093600	-0.43848100	0.64246800
N	0.67812200	-0.51234600	0.56919000

Phe

O	2.94915300	2.23286300	-1.17342300
O	2.68449000	2.87131600	0.97339600
N	0.45341800	0.89648800	0.44987400
N	-1.65067900	0.62810300	0.37016400
C	-0.48082200	0.00559700	0.02905900
C	-1.44251200	1.85849000	0.98474400
H	-2.24743800	2.49813000	1.30636100
C	-0.10294800	2.02243800	1.03321700
H	0.52640200	2.81860700	1.39839700
C	1.91965400	0.70148800	0.37190800
H	2.25325600	0.44085000	1.38102100
C	2.59885100	2.08205100	0.00992600
C	2.26492900	-0.42267200	-0.59898700
H	1.52893200	-1.22155900	-0.49766100
H	2.18422100	-0.01057700	-1.60778700
C	3.64887900	-0.97288300	-0.37620100
C	3.82825300	-2.19236100	0.28076800
H	2.95460700	-2.73647800	0.62666100
C	5.09790000	-2.71944200	0.49287800
H	5.20975500	-3.66988600	1.00487300
C	6.21980200	-2.03021700	0.04764700
H	7.21264500	-2.43656200	0.21027700
C	6.05547900	-0.81298200	-0.60625500
H	6.92470600	-0.26357600	-0.95298500
C	4.78593900	-0.28804700	-0.81646300
H	4.64633500	0.66926800	-1.30763400
C	-2.93348600	0.07599700	0.10290900
C	-3.45648700	0.15547100	-1.19208100
C	-4.72235300	-0.37563800	-1.42737300
H	-5.13562500	-0.31512000	-2.43020300
C	-5.46732800	-0.97795300	-0.41667900
C	-4.91484400	-1.04502700	0.85847300
H	-5.47572400	-1.51939100	1.65881800
C	-3.64993000	-0.53028200	1.13808100
C	-2.66347100	0.78906700	-2.29569900
H	-2.37980400	1.81349300	-2.04234900
H	-3.23500700	0.80449200	-3.22533300
H	-1.73097600	0.24340300	-2.45599700
C	-6.81706200	-1.57405300	-0.70668200
H	-7.35376700	-0.99602700	-1.46247900
H	-7.43629400	-1.61378400	0.19194700
H	-6.72199200	-2.59706700	-1.08539300
C	-3.05633000	-0.64714400	2.51163700
H	-2.05317300	-1.07590200	2.45906900
H	-3.67788100	-1.27846200	3.14900600
H	-2.95415800	0.32919200	2.99238600

Complexes $[Ni(CO)_2(\kappa^2\text{-AA})]^-$.

Val

Ni	-0.58338400	1.41357800	0.10189200
O	-2.39684500	1.42914000	-1.04335500
O	-4.02246700	0.40095000	-2.20006200
N	-1.51622200	-1.28944900	-0.54524100
N	0.61146400	-1.34205900	-0.34473100
C	-0.45940200	-0.49927100	-0.21539900

C	-1.11861200	-2.56754900	-0.87993600
H	-1.82037900	-3.32955200	-1.17321600
C	0.22634000	-2.60933900	-0.75489700
H	0.93195700	-3.40592200	-0.91694100
C	1.96757800	-0.95247400	-0.13761700
C	2.48955100	-0.96024600	1.15738000
C	3.82454200	-0.60255800	1.32846100
H	4.23996000	-0.59884900	2.33190300
C	4.62951300	-0.23692500	0.25338900
C	4.07113700	-0.23376300	-1.02145400
H	4.67843100	0.06742200	-1.86977600
C	2.74064400	-0.58137500	-1.24023100
C	1.62257200	-1.31014800	2.32937100
H	0.81063900	-0.58428000	2.42336000
H	2.20205500	-1.31058500	3.25384500
H	1.16143700	-2.29380200	2.20799500
C	6.05302600	0.19505400	0.46970200
H	6.11166400	1.27870400	0.61339200
H	6.68101600	-0.05530700	-0.38817800
H	6.48302000	-0.27699600	1.35575400
C	2.13653000	-0.51970700	-2.61164800
H	1.79669400	-1.50228100	-2.95016600
H	2.85854600	-0.13757900	-3.33443900
H	1.26381100	0.13793800	-2.60951300
C	-2.91521700	-0.85303100	-0.52163400
H	-3.48683800	-1.64081300	-1.01832600
C	-3.12364300	0.45179900	-1.35120700
C	-3.42225000	-0.68275900	0.91924800
H	-2.80086800	0.09855400	1.36909200
C	-4.87382700	-0.21296900	0.92592300
H	-4.99220700	0.72809000	0.38786000
H	-5.21944300	-0.06934200	1.95411800
H	-5.52872200	-0.94971500	0.44826600
C	-3.26592800	-1.96432600	1.73339500
H	-3.86959800	-2.77581000	1.30931500
H	-3.60139400	-1.80780000	2.76299300
H	-2.22706000	-2.29959400	1.77123200
C	0.58185900	2.41028800	-0.76569400
C	-0.74651800	1.96908000	1.75640600
O	1.41037000	3.08603400	-1.20407300
O	-0.68005900	2.35002800	2.84835300

Leu

Ni	-0.24063300	1.49408400	0.65018800
O	-1.89767100	2.29361100	-0.44000400
O	-3.71931000	2.14566700	-1.74310200
N	-1.44705700	-0.46620000	-1.15881400
N	0.62808400	-0.93612000	-0.94807400
C	-0.33389800	-0.08253500	-0.47866300
C	-1.18544400	-1.50659200	-2.02741300
H	-1.94608900	-1.93804400	-2.65552300
C	0.12516100	-1.81008000	-1.89933200
H	0.73497300	-2.55151100	-2.38627200
C	1.99679000	-0.89883100	-0.54943900
C	2.38507900	-1.55615200	0.61959800
C	3.73244800	-1.52874500	0.97073300
H	4.04539000	-2.03147000	1.88111400
C	4.67894000	-0.86411900	0.19630600
C	4.25214000	-0.21358100	-0.95771300
H	4.97305800	0.32693100	-1.56376500
C	2.91521000	-0.21178300	-1.34669100
C	1.37019600	-2.23856400	1.48668200
H	0.66462300	-1.50398300	1.88362600
H	1.85336700	-2.74842800	2.32158400
H	0.78709300	-2.97085600	0.92232800
C	6.11912400	-0.80566100	0.62314100
H	6.39294000	-1.67604500	1.22331600
H	6.30748400	0.08519300	1.23081200
H	6.78942800	-0.76140900	-0.23813400
C	2.46027300	0.54077700	-2.56173000
H	2.03639100	-0.12611200	-3.31751100
H	3.29126100	1.08577800	-3.01137500
H	1.67978400	1.25609400	-2.29105500
C	-2.77896200	0.12071100	-0.97903100
H	-3.38132800	-0.24018800	-1.81293700
C	-2.78648300	1.67839900	-1.07769800
C	-3.39786400	-0.29742500	0.35528500

H	-2.75374400	0.09690600	1.14652200
H	-4.36031000	0.22027000	0.43956100
C	-3.60608700	-1.80000600	0.56276600
H	-2.65268000	-2.30506900	0.36212700
C	-3.98067800	-2.08049600	2.01675000
H	-3.21257100	-1.71020000	2.69990200
H	-4.10982200	-3.15251400	2.19749000
H	-4.92168900	-1.58360600	2.27646800
C	-4.66035300	-2.37980700	-0.37808400
H	-5.63233400	-1.90562000	-0.20532000
H	-4.78074200	-3.45642500	-0.22144100
H	-4.40560100	-2.22512100	-1.42913500
C	1.13668400	2.55578400	0.37044100
C	-0.52004600	1.29471600	2.36918400
O	2.08992200	3.20683100	0.31565000
O	-0.53065800	1.14154600	3.51745800

lLe

Ni	-0.24063300	1.49408400	0.65018800
O	-1.89767100	2.29361100	-0.44000400
O	-3.71931000	2.14566700	-1.74310200
N	-1.44705700	-0.46620000	-1.15881400
N	0.62808400	-0.93612000	-0.94807400
C	-0.33389800	-0.08253500	-0.47866300
C	-1.18544400	-1.50659200	-2.02741300
H	-1.94608900	-1.93804400	-2.65552300
C	0.12516100	-1.81008000	-1.89933200
H	0.73497300	-2.55151100	-2.38627200
C	1.99679000	-0.89883100	-0.54943900
C	2.38507900	-1.55615200	0.61959800
C	3.73244800	-1.52874500	0.97073300
H	4.04539000	-2.03147000	1.88111400
C	4.67894000	-0.86411900	0.19630600
C	4.25214000	-0.21358100	-0.95771300
H	4.97305800	0.32693100	-1.56376500
C	2.91521000	-0.21178300	-1.34669100
C	1.37019600	-2.23856400	1.48668200
H	0.66462300	-1.50398300	1.88362600
H	1.85336700	-2.74842800	2.32158400
H	0.78709300	-2.97085600	0.92232800
C	6.11912400	-0.80566100	0.62314100
H	6.39294000	-1.67604500	1.22331600
H	6.30748400	0.08519300	1.23081200
H	6.78942800	-0.76140900	-0.23813400
C	2.46027300	0.54077700	-2.56173000
H	2.03639100	-0.12611200	-3.31751100
H	3.29126100	1.08577800	-3.01137500
H	1.67978400	1.25609400	-2.29105500
C	-2.77896200	0.12071100	-0.97903100
H	-3.38132800	-0.24018800	-1.81293700
C	-2.78648300	1.67839900	-1.07769800
C	-3.39786400	-0.29742500	0.35528500
H	-2.75374400	0.09690600	1.14652200
H	-4.36031000	0.22027000	0.43956100
C	-3.60608700	-1.80000600	0.56276600
H	-2.65268000	-2.30506900	0.36212700
C	-3.98067800	-2.08049600	2.01675000
H	-3.21257100	-1.71020000	2.69990200
H	-4.10982200	-3.15251400	2.19749000
H	-4.92168900	-1.58360600	2.27646800
C	-4.66035300	-2.37980700	-0.37808400
H	-5.63233400	-1.90562000	-0.20532000
H	-4.78074200	-3.45642500	-0.22144100
H	-4.40560100	-2.22512100	-1.42913500
C	1.13668400	2.55578400	0.37044100
C	-0.52004600	1.29471600	2.36918400
O	2.08992200	3.20683100	0.31565000
O	-0.53065800	1.14154600	3.51745800

Phe

Ni	0.19440800	1.35528600	-0.05561300
O	-1.60303700	1.33047500	-1.25236000
O	-2.85834800	0.16264100	-2.70462600
N	-0.65281400	-1.39064800	-0.66627700
N	1.44728100	-1.40275500	-0.27489700
C	0.36469100	-0.56624800	-0.29841400

C	1.10653800	-2.70120900	-0.62195400
H	1.82944600	-3.49748600	-0.66720800
C	-0.22247800	-2.68623000	-0.86651300
H	-0.89044500	-3.47419400	-1.17035100
C	-2.05039100	-0.96948300	-0.77987300
H	-2.58060000	-1.78077200	-1.28008500
C	-2.17800400	0.29692600	-1.68411200
C	-2.62772500	-0.73986200	0.62534900
H	-2.41669500	-1.62430200	1.23626300
H	-2.07885800	0.10035300	1.05965400
C	-4.10548900	-0.46436000	0.63858900
C	-5.01348400	-1.45098000	1.02468900
H	-4.64029200	-2.42702600	1.32071600
C	-6.38172200	-1.20302300	1.04312100
H	-7.06880600	-1.98481400	1.34970000
C	-6.86518700	0.04497900	0.67003100
H	-7.93138300	0.24403200	0.68103500
C	-5.97004500	1.03594400	0.28005200
H	-6.33740100	2.01128100	-0.01964200
C	-4.60427500	0.78638900	0.26532600
H	-3.90828400	1.55594400	-0.05041800
C	2.77676200	-0.98474100	0.02948600
C	3.63399300	-0.64082000	-1.01822000
C	4.93578500	-0.26113700	-0.70197700
H	5.60819300	0.01907700	-1.50724400
C	5.38504100	-0.20916000	0.61439400
C	4.49884800	-0.55250200	1.63139000
H	4.82885000	-0.50707800	2.66503100
C	3.18829600	-0.93949400	1.36280900
C	3.14817700	-0.64601600	-2.43712000
H	2.84599800	-1.64673000	-2.75778700
H	3.92610100	-0.28852300	-3.11289900
H	2.27349100	0.00078600	-2.53936300
C	6.77876700	0.25556900	0.93256200
H	7.48035400	-0.01454900	0.14025000
H	7.13940000	-0.17622900	1.86861900
H	6.80916500	1.34457000	1.03971000
C	2.23175700	-1.26642700	2.47016500
H	1.40188800	-0.55517400	2.47082800
H	2.73103700	-1.22249700	3.43921700
H	1.79998200	-2.26307100	2.34692100
C	1.35942400	2.35050500	-0.92675000
C	-0.01905500	1.95612000	1.57745000
O	0.01954600	2.37239600	2.65714200
O	2.18594200	3.02496100	-1.36895800

Species of the non-catalyzed reaction between PhCHO and $PhSiH_3$

PhCHO

C	-0.35399000	1.28375200	0.00000100
C	0.53145400	0.20690200	-0.00000100
C	0.04054000	-1.10071400	0.00000000
C	-1.32614100	-1.32287200	0.00000300
C	-2.20801700	-0.24313700	0.00000400
C	-1.72436000	1.06003900	0.00000400
H	0.03608400	2.29671900	0.00000100
H	0.74791800	-1.92145400	-0.00000100
H	-1.71189300	-2.33543400	0.00000300
H	-3.27723400	-0.42101200	0.00000600
H	-2.41337900	1.89604300	0.00000500
C	1.98521100	0.46304200	-0.00000300
H	2.26382500	1.53768400	-0.00000700
O	2.83581300	-0.39182800	-0.00000700

$PhSiH_3$

Si	-2.33985700	-0.00000100	0.00578800
H	-2.85062800	-1.21608300	-0.68250600
H	-2.86757200	-0.00002500	1.39861200
H	-2.85060600	1.21611800	-0.68245700
C	-0.46390400	-0.00000700	-0.01295800
C	0.25551900	-1.20034000	-0.00997300

C	0.25550900	1.20033400	-0.00997400
C	1.64517300	-1.20241000	0.00316000
H	-0.27256800	-2.14849400	-0.02250900
C	1.64516300	1.20241600	0.00316100
H	-0.27258600	2.14848200	-0.02251000
C	2.34210600	0.00000600	0.01064200
H	2.18429700	-2.14285500	0.00380600
H	2.18427900	2.14286500	0.00380700
H	3.42598800	0.00001000	0.01836600

Aduct PhCHO-$PhSiH_3$

C	4.28548300	1.35257000	-0.00020600
C	3.59481700	0.14122000	-0.00003300
C	4.29946800	-1.06497600	0.00016200
C	5.68390900	-1.05291000	0.00018200
C	6.37049500	0.16046400	0.00000800
C	5.67382700	1.36336200	-0.00018600
H	3.72989300	2.28499500	-0.00035600
H	3.74122500	-1.99355900	0.00029400
H	6.23525000	-1.98565700	0.00033300
H	7.45438200	0.16577900	0.00002500
H	6.21173700	2.30368600	-0.00032000
C	2.12067600	0.14917000	-0.00005600
H	1.66019600	1.15841000	-0.00021400
O	1.42685600	-0.83908300	0.00008100
H	-0.98238100	0.88548200	-0.00018600
Si	-1.69594000	-0.42265200	0.00003200
H	-1.33754200	-1.17670000	1.22765400
H	-1.33757900	-1.17709000	-1.22736100
C	-3.55432800	-0.11907700	0.00001200
C	-4.26540100	0.00688900	-1.19886200
C	-4.26535200	0.00731300	1.19887000
C	-5.63252000	0.25818000	-1.20205000
H	-3.74725600	-0.09718000	-2.14719800
C	-5.63247200	0.25860600	1.20202400
H	-3.74717000	-0.09641900	2.14722300
C	-6.31861500	0.38551000	-0.00002100
H	-6.16356900	0.35034900	-2.14281100
H	-6.16348200	0.35110900	2.14277400
H	-7.38530400	0.57866100	-0.00003400

Transition state PhCHO-$PhSiH_3$

C	-2.75834000	-0.54280600	1.36508500
C	-2.33995000	0.31455500	0.34857500
C	-2.94810600	0.26150400	-0.90327500
C	-3.96920400	-0.64899900	-1.13597600
C	-4.38023300	-1.50982800	-0.12299700
C	-3.77557500	-1.45614400	1.12918900
H	-2.28691900	-0.49146700	2.34164200
H	-2.61748000	0.95381900	-1.66803100
H	-4.44935400	-0.68703100	-2.10670100
H	-5.17790800	-2.22014900	-0.30701000
H	-4.10189600	-2.12170900	1.91943800
C	-1.26378300	1.31541800	0.59860500
H	-1.10704300	1.50931200	1.67452200
O	-1.04042000	2.26681600	-0.24502300
H	-0.11548900	0.44372100	0.53507400
Si	0.82102400	1.39605300	-0.39544900
H	1.31301000	2.64288900	0.23883600
H	0.41531300	1.16485600	-1.79996900
C	2.32991700	0.26283900	-0.18860600
C	2.47436600	-0.89948800	-0.95682300
C	3.33189100	0.56118100	0.74243700
C	3.57832900	-1.72928900	-0.80680800
H	1.71570800	-1.15631000	-1.69120600
C	4.43901900	-0.26443800	0.89980100
H	3.25135600	1.46018400	1.34753500
C	4.56191100	-1.41214300	0.12456800
H	3.67582700	-2.62113300	-1.41573600
H	5.20757200	-0.01292500	1.62213600
H	5.42487400	-2.05749100	0.24328100

$PhSiH_2OCH_2Ph$

C	3.95613800	-0.77820800	0.24363600
C	2.63610200	-0.40411800	-0.00782900
C	2.36032700	0.91192400	-0.36058700
C	3.39113500	1.84135000	-0.46075200
C	4.70387900	1.46475100	-0.21063600
C	4.98414900	0.14847500	0.14280200
H	4.18268600	-1.80316700	0.52198800
H	1.33454600	1.19732400	-0.55456500
H	3.16428100	2.86491800	-0.73673900
H	5.50523200	2.19012000	-0.28894900
H	6.00534100	-0.15560600	0.34196600
C	1.54438900	-1.43732800	0.09697500
H	1.59980600	-1.92248200	1.08156500
O	0.27485000	-0.85790500	-0.09316200
H	1.71728000	-2.21787200	-0.65692400
Si	-1.16311900	-1.65248600	0.16098500
H	-1.08809200	-2.32535900	1.49066200
H	-1.39804900	-2.69337600	-0.87986500
C	-2.52635400	-0.38630300	0.08319400
C	-3.64737000	-0.59999000	-0.72533100
C	-2.47079200	0.78620500	0.84682100
C	-4.68460900	0.32503500	-0.76828300
H	-3.71203900	-1.49640400	-1.33381500
C	-3.50287800	1.71380300	0.80266100
H	-1.60972900	0.98064700	1.47762800
C	-4.61226200	1.48276800	-0.00422600
H	-5.54552600	0.14440600	-1.40160200
H	-3.44359500	2.61802900	1.39754000
H	-5.41839400	2.20668500	-0.03806000

Leu_2Ni

Ni	-0.07804400	-0.10034300	-0.15799000
O	-1.35836900	-0.09112100	-1.51077300
O	-3.11358200	-0.86250100	-2.62837700
N	1.23963500	-2.79898500	-0.44696800
N	-0.87398300	-2.77827200	-0.78062100
C	0.15925400	-1.98306300	-0.44289400
C	-0.46078700	-4.07633000	-0.99153100
H	-1.14026200	-4.86315700	-1.26931200
C	0.87530700	-4.09028000	-0.78397000
H	1.59720200	-4.88527800	-0.85171000
C	-2.23960900	-2.27968000	-0.94458600
H	-2.77683400	-3.02055500	-1.53485300
C	-2.24710900	-0.98404500	-1.78100000
C	-2.93173400	-2.05909100	0.40191000
H	-2.34141900	-1.32938300	0.96610700
H	-3.89941700	-1.58839000	0.19913100
C	2.60875400	-2.39673100	-0.28529000
C	3.29073700	-1.91790000	-1.40491300
C	3.22052000	-2.53388800	0.96288100
C	4.63064600	-1.56788100	-1.24716900
C	4.56017400	-2.17536300	1.06568000
C	5.28103800	-1.69155300	-0.02333200
H	5.17684000	-1.19185700	-2.10650800
H	5.04466600	-2.25457000	2.03309900
O	1.16966400	-0.10098600	1.22815100
O	2.87045200	0.72149200	2.39036000
N	-1.32316200	2.63881200	0.17870300
N	0.80979200	2.55541500	0.37071900
C	-0.27069700	1.79372700	0.10504300
C	0.44738700	3.86355400	0.61559400
H	1.15361900	4.63838700	0.84948400
C	-0.89829100	3.91647600	0.49301100
H	-1.58794800	4.73519800	0.60167000
C	2.15310500	1.95686800	0.45805600
H	2.35352000	1.50892400	-0.51955100
C	2.08100800	0.77903500	1.46689200
C	3.23618800	2.96440900	0.79242400
H	2.93295200	3.54070200	1.67227700
H	4.09918000	2.38428000	1.12762700
C	-2.71112600	2.28172300	0.08607800
C	-3.36793500	2.39728500	-1.14135700
C	-3.36435800	1.87451400	1.25024000

C	-4.72227800	2.08345200	-1.17751200
C	-4.72132700	1.57029100	1.15941000
C	-5.41488800	1.66777800	-0.04293700
H	-5.24307000	2.14690800	-2.12704400
H	-5.24585300	1.25055200	2.05433300
C	-6.87362800	1.31903200	-0.12826500
H	-7.28381800	1.07486600	0.85271800
H	-7.45478800	2.14814700	-0.53982000
H	-7.02974200	0.45789000	-0.78380900
C	-2.63547100	2.79218800	-2.38696800
H	-2.01763900	3.68044900	-2.23547900
H	-1.98334200	1.97047500	-2.69227300
H	-3.33663700	2.99341700	-3.19676400
C	-2.63683100	1.76571500	2.55992100
H	-1.78627600	1.08272300	2.49298500
H	-2.24072600	2.73300900	2.88114200
H	-3.30555600	1.40219800	3.34042600
C	2.45059400	-2.98858000	2.16502600
H	1.74739500	-2.20398900	2.45494900
H	1.88176100	-3.90054500	1.96933000
H	3.12204800	-3.17477100	3.00307700
C	6.72585500	-1.31007900	0.13024400
H	7.33838800	-2.18155000	0.37764300
H	7.12273800	-0.87282000	-0.78703600
H	6.85495800	-0.58382300	0.93662600
C	2.61040500	-1.77764300	-2.73684800
H	1.76680300	-1.08422500	-2.68647700
H	3.31002500	-1.40933100	-3.48750100
H	2.21293000	-2.73367600	-3.08806900
C	3.65905300	3.89843800	-0.35011800
H	2.76485300	4.34871900	-0.79930600
C	4.52628300	5.02894400	0.19869100
H	4.83994800	5.71038900	-0.59601800
H	3.99422500	5.61550300	0.95286500
H	5.42952800	4.62950400	0.67032800
C	4.40060100	3.14769200	-1.45466000
H	5.31540800	2.69212700	-1.06309200
H	3.79636500	2.35236000	-1.89709000
H	4.68497900	3.82688700	-2.26228600
C	-3.13812700	-3.31574300	1.25240000
H	-2.16974800	-3.82157100	1.35523600
C	-3.60272100	-2.92321400	2.65321000
H	-4.56138000	-2.39647800	2.61143200
H	-3.73606500	-3.80446500	3.28583700
H	-2.88033900	-2.26510600	3.14214600
C	-4.12619300	-4.29129500	0.61670900
H	-5.10954700	-3.82495300	0.50092100
H	-3.80727200	-4.62986700	-0.37213500
H	-4.25150400	-5.18005500	1.24031700

Leu$_2$Ni with a dissociated carboxylate arm

Ni	-0.05126100	0.12886000	-0.01488400
O	2.31575200	-3.58461200	1.46666500
O	3.63271300	-1.74261200	1.51704400
N	-1.97553100	-2.24798000	0.61597500
N	0.01792600	-2.10211200	1.38453100
C	-0.88894400	-1.45550100	0.64099100
C	-0.46527800	-3.30538100	1.84315300
H	0.13943700	-3.99063100	2.40757800
C	-1.72997500	-3.39462100	1.35929500
H	-2.46974700	-4.16973700	1.45848300
C	1.29898200	-1.42156100	1.57839900
H	1.45867300	-0.79147500	0.64585000
C	2.57430300	-2.37848600	1.50198700
C	1.29905100	-0.50758400	2.80614300
C	-3.18758200	-1.99753000	-0.11036400
C	-4.19526700	-1.24418300	0.49232600
C	-3.32000900	-2.53169800	-1.39298000
C	-5.36653600	-1.03501900	-0.22830200
C	-4.51084300	-2.29346500	-2.07332000
C	-5.54185600	-1.54624300	-1.51101100
H	-6.15819500	-0.44603100	0.22309800
H	-4.63110300	-2.69988800	-3.07242600
O	-1.57351000	0.95410700	-0.61823300
O	-2.93105600	2.68196000	-0.84274600

N	2.07403300	1.63421300	-1.47015800
N	0.51504400	2.84874900	-0.63348000
C	0.97893700	1.58791400	-0.68579100
C	1.30898800	3.69102900	-1.38352700
H	1.12320700	4.74472700	-1.48043500
C	2.29520300	2.92413600	-1.90761700
H	3.12757300	3.17675300	-2.54079300
C	-0.75316200	3.14708300	0.04935100
H	-0.61829900	2.83946100	1.09093000
C	-1.85549000	2.21971000	-0.53197200
C	-1.12926300	4.61565900	-0.00043500
C	2.82537600	0.47700900	-1.87635000
C	3.99492400	0.13982300	-1.19528100
C	2.33628800	-0.27227000	-2.95528400
C	4.66713100	-1.00981000	-1.60819100
C	3.04775400	-1.40642100	-3.32478500
C	4.20746700	-1.79786300	-2.65470000
H	5.55501600	-1.30978100	-1.06310000
H	2.68388100	-2.00440300	-4.15408300
C	4.91735900	-3.06768200	-3.02343300
H	5.99906400	-2.96274400	-2.92358900
H	4.60582100	-3.87880600	-2.35873000
H	4.69368800	-3.36960500	-4.04795600
C	4.51656200	0.91607800	-0.02307300
H	5.58555200	1.10784100	-0.13911400
H	4.01224000	1.87292100	0.11004600
H	4.37963200	0.30848200	0.87644300
C	1.09292800	0.13209900	-3.69594900
H	0.21020600	0.12545300	-3.05079000
H	1.17887100	1.14215600	-4.10575300
H	0.90685700	-0.55001300	-4.52552100
C	-2.21318500	-3.32078500	-2.03025200
H	-1.30801000	-2.71717300	-2.13413200
H	-1.94254800	-4.19795300	-1.43764800
H	-2.50858600	-3.66187200	-3.02249700
C	-6.79885200	-1.26466600	-2.28267400
H	-6.97899300	-2.02507500	-3.04426000
H	-7.66980600	-1.22603000	-1.62580000
H	-6.72822800	-0.29778100	-2.79002300
C	-4.01546100	-0.64900500	1.85735800
H	-3.28804600	0.16599800	1.82367100
H	-4.95742800	-0.24382600	2.22701100
H	-3.65114200	-1.38349300	2.57909100
H	2.27560700	-0.01596000	2.82021100
H	0.53980600	0.27154300	2.66232700
H	-1.08862700	4.96217200	-1.03812700
H	-2.18663900	4.66984800	0.26865000
C	-0.31954000	5.54476100	0.91459500
H	0.75174000	5.37708400	0.74562300
C	-0.62464000	7.00025400	0.56847800
H	-0.05556500	7.68506200	1.20157800
H	-0.38170300	7.22679700	-0.47332100
H	-1.68712000	7.21807400	0.71362900
C	-0.60114600	5.27851200	2.39220600
H	-1.65962200	5.43915000	2.61871600
H	-0.34650300	4.25893700	2.69182000
H	-0.01953500	5.95311700	3.02487700
C	1.03637000	-1.17494700	4.16365200
H	0.12223000	-1.77581400	4.07670500
C	0.77042700	-0.08899700	5.20591700
H	0.55710600	-0.53024600	6.18256400
H	1.64416300	0.56026400	5.32127000
H	-0.08068600	0.53964600	4.92880600
C	2.17129300	-2.08674700	4.62568600
H	3.10704700	-1.52706400	4.70763200
H	1.94047600	-2.50292700	5.61030700
H	2.34816200	-2.91768900	3.94254400

Leu_2Ni conformer

Ni	-0.00160400	-0.00219000	-0.67852000
O	-3.42910600	0.67553800	-2.25643800
O	-1.79815200	0.47189100	-0.76995400
N	0.03905700	-2.91791100	-0.05124900
N	-1.63601500	-2.31661400	-1.25171000
C	-0.52960200	-1.84106100	-0.64318600

C	-1.75076000	-3.68087800	-1.06161100
H	-2.55091200	-4.26462400	-1.47712600
C	-0.69850800	-4.05773700	-0.30427200
H	-0.41216600	-5.01920100	0.08480000
C	-2.56703500	-1.50028500	-2.04295800
H	-2.20920200	-1.50703800	-3.07805700
C	-2.60160400	0.00157600	-1.66021800
C	-3.97986300	-2.10379000	-2.06401000
C	1.17560900	-2.91369100	0.82773700
C	2.41205400	-3.35697400	0.35552800
C	0.97739700	-2.52408800	2.15519300
C	3.46953900	-3.39429200	1.26244200
C	2.06924400	-2.57043500	3.01682600
C	3.32306700	-2.99963300	2.58821800
H	4.43895800	-3.73419600	0.91214900
H	1.93140500	-2.27301600	4.05170100
O	1.79289000	-0.47881700	-0.78598300
O	3.42119700	-0.68133300	-2.27447200
N	-0.04000100	2.91416900	-0.05752500
N	1.63180500	2.31195900	-1.26219200
C	0.52589000	1.83707600	-0.65187400
C	1.74664200	3.67687100	-1.07293600
H	2.54659200	4.26027500	-1.48952500
C	0.69327200	4.05503000	-0.31782100
H	0.40577500	5.01701500	0.06917100
C	2.56538300	1.49636700	-2.05119300
H	2.20998500	1.50696000	-3.08693100
C	2.59468400	-0.00770800	-1.67632900
C	3.98037200	2.09845900	-2.06447100
H	3.95344900	3.02279400	-2.65334000
C	-1.17282800	2.91135100	0.82642500
C	-2.40854200	3.36142800	0.35931700
C	-0.97200100	2.51804200	2.15250800
C	-3.46297200	3.40183900	1.26958700
C	-2.06102200	2.56724800	3.01762900
C	-3.31417200	3.00328200	2.59398400
H	-4.43166700	3.74792000	0.92337100
H	-1.92137500	2.26662900	4.05133300
C	-4.48233400	3.02034400	3.53864400
H	-4.16033200	3.17970800	4.56941000
H	-5.19379600	3.80595900	3.27821700
H	-5.02045100	2.06786900	3.50595700
C	-2.63062300	3.74142400	-1.07279700
H	-1.77718500	4.26929900	-1.50127400
H	-2.80302800	2.83628000	-1.66443000
H	-3.51015100	4.38008500	-1.16729000
C	0.37624200	2.07274700	2.64328400
H	0.74005600	1.20045000	2.09546700
H	1.12497400	2.86070800	2.52077400
H	0.33159600	1.81530300	3.70179600
C	-0.37136300	-2.08554600	2.65062500
H	-0.73585100	-1.20767800	2.11208400
H	-1.11945700	-2.87260900	2.51932400
H	-0.32702400	-1.83937800	3.71184200
C	4.49440200	-3.01285000	3.52901700
H	4.17664200	-3.17640800	4.56044600
H	5.20913500	-3.79406500	3.26434200
H	5.02740500	-2.05748300	3.49687100
C	2.63384500	-3.72945700	-1.07851900
H	2.80924100	-2.82123700	-1.66455800
H	3.51175700	-4.36988500	-1.17578200
H	1.77937800	-4.25240100	-1.51094500
H	-4.57956000	-1.39953800	-2.64562100
H	-3.94852100	-3.03083500	-2.64876600
H	4.58404300	1.39327000	-2.64048400
C	-4.69762100	-2.39781900	-0.74026300
H	-4.07331300	-3.07857300	-0.14633200
C	-4.96789300	-1.15811900	0.11053600
H	-5.52183600	-0.40699200	-0.45801100
H	-5.56649000	-1.43482700	0.98256200
H	-4.05845100	-0.68524300	0.47911800
C	-6.00898900	-3.11657600	-1.05103100
H	-6.65562300	-2.49070300	-1.67398800
H	-5.84713200	-4.05742400	-1.58457700
H	-6.55559200	-3.34464900	-0.13320200
C	4.68801500	2.39569100	-0.73454800
H	4.04847800	3.05262400	-0.13069800
C	5.97918300	3.15443800	-1.03425700

H	5.78814300	4.09863000	-1.55262100
H	6.52101700	3.38361900	-0.11355300
H	6.64257900	2.55717500	-1.66763600
C	4.99464900	1.15413400	0.10093600
H	5.58603000	0.43422100	-0.47029900
H	5.56937300	1.44025100	0.98614400
H	4.09892200	0.64438100	0.45338400

Val_2Ni

Ni	0.05766700	-0.16920600	0.06577000
O	1.42632700	-0.74528400	1.18900400
O	2.91315200	-2.17302000	2.00755300
N	-1.90939500	-2.45734900	0.10122900
N	0.14979300	-3.03531900	0.13959700
C	-0.65171500	-1.95488000	0.07334400
C	-0.58045700	-4.20216500	0.20351800
H	-0.11809900	-5.17219200	0.25895400
C	-1.88209400	-3.83832100	0.18254700
H	-2.78475600	-4.42221200	0.22731300
C	1.60744500	-2.94189300	0.17928600
H	1.97495800	-3.90205800	0.54516300
C	2.02602600	-1.88618400	1.22368200
C	2.20800200	-2.66702100	-1.21144200
H	1.86088300	-1.67242900	-1.51784300
C	-3.13258400	-1.71076800	0.19730100
C	-3.56253300	-1.31239900	1.46507700
C	-3.87960900	-1.46827600	-0.95683600
C	-4.78531100	-0.65162700	1.55696500
C	-5.09685500	-0.80993800	-0.80951200
C	-5.56638700	-0.39474500	0.43332300
H	-5.13802300	-0.33963100	2.53507600
H	-5.68398800	-0.60254800	-1.69785000
O	-1.26289800	0.39709000	-1.10673000
O	-2.81234200	1.75110100	-1.90818600
N	1.88740900	2.23304800	0.29914100
N	-0.21108500	2.67121200	0.20293300
C	0.67345600	1.64915400	0.17251200
C	0.43662000	3.87868900	0.37325200
H	-0.07302600	4.82091800	0.44091700
C	1.75765500	3.60297000	0.42360400
H	2.61260700	4.24821500	0.52581100
C	-1.66801400	2.45258300	0.08996900
H	-1.96245800	1.90628900	0.99306200
C	-1.94963400	1.48499400	-1.09108700
C	-2.45860700	3.76760600	0.07217100
H	-2.07791100	4.35383100	0.91864500
C	3.17617500	1.60814300	0.18654700
C	3.88608300	1.28736800	1.34533100
C	3.71170900	1.43589900	-1.09160100
C	5.17047700	0.77387500	1.19110800
C	5.00191400	0.92083500	-1.19049000
C	5.74526400	0.58434400	-0.06266700
H	5.73024800	0.50437400	2.08047400
H	5.43547600	0.78367600	-2.17609600
C	7.12219000	-0.00171900	-0.19224200
H	7.56503600	0.22943700	-1.16242400
H	7.78937400	0.37441600	0.58584500
H	7.08921700	-1.09105400	-0.09333100
C	3.28038000	1.44918300	2.70582400
H	2.85913000	2.44686100	2.85150000
H	2.47745100	0.71874700	2.82724800
H	4.02629200	1.27407800	3.48090600
C	2.93339900	1.80230400	-2.32298800
H	2.00522900	1.23027100	-2.39692000
H	2.65436000	2.85957300	-2.32235200
H	3.52346700	1.61158600	-3.21965300
C	-3.37058900	-1.85136000	-2.31274400
H	-2.52903000	-1.20453300	-2.57274600
H	-3.02632700	-2.88767600	-2.34580000
H	-4.14816500	-1.72248600	-3.06549000
C	-6.87126500	0.33964700	0.55216600
H	-7.61952300	-0.06680500	-0.13110100
H	-7.26994200	0.28369800	1.56643200
H	-6.74396200	1.39751200	0.30348000
C	-2.74295500	-1.58952800	2.69299800

H	-1.75964300	-1.11571300	2.63505300
H	-3.24912700	-1.21658400	3.58364900
H	-2.57005400	-2.66065500	2.82796800
C	1.72604400	-3.68381000	-2.24205600
H	2.16322000	-3.46455600	-3.21887400
H	2.03351700	-4.69805600	-1.96577300
H	0.64064800	-3.67499500	-2.35747400
C	3.73135700	-2.65403800	-1.13405400
H	4.11069500	-3.63012000	-0.81607300
H	4.15444300	-2.43380100	-2.11675500
H	4.09964400	-1.90829500	-0.42991200
C	-2.30399500	4.59775200	-1.20451600
H	-2.80949700	4.10579700	-2.03377300
H	-2.74818600	5.58599700	-1.05792200
H	-1.26069800	4.74251700	-1.49344000
C	-3.93474200	3.50081700	0.36652200
H	-4.38135200	2.91253700	-0.43487300
H	-4.06392300	2.96133900	1.30886400
H	-4.47496300	4.44731000	0.44626700

ILe$_2$Ni

Ni	-0.14013300	-0.17803100	-0.15422000
O	-1.52701000	-0.46827100	-1.36271800
O	-3.14411200	-1.61702400	-2.35485100
N	1.50634100	-2.69988200	-0.35252500
N	-0.60926300	-2.98784900	-0.48328700
C	0.32651600	-2.03614900	-0.30270800
C	-0.03923500	-4.23240200	-0.64179000
H	-0.62481100	-5.12203600	-0.79508200
C	1.29797400	-4.05164800	-0.56204200
H	2.11574000	-4.74625300	-0.64268800
C	-2.03899200	-2.69187900	-0.54601900
H	-2.52122000	-3.56103700	-0.99613700
C	-2.26764600	-1.51272600	-1.51536400
C	-2.64821600	-2.43619500	0.84654300
H	-2.18049100	-1.52202000	1.23597400
C	2.82028300	-2.12013900	-0.35390800
C	3.33983700	-1.66951400	-1.56933300
C	3.55199700	-2.07837900	0.83452500
C	4.63942400	-1.16754600	-1.57255700
C	4.84685900	-1.57235900	0.77594600
C	5.40894400	-1.11739200	-0.41356500
H	5.05948200	-0.81196700	-2.50825200
H	5.42186800	-1.51460300	1.69403700
O	1.19811300	0.10423000	1.09894700
O	2.88677400	1.16386900	2.04964600
N	-1.62504200	2.46161100	-0.21940800
N	0.50835400	2.60023700	-0.03440300
C	-0.50513500	1.70931600	-0.11655100
C	0.03416500	3.89480300	-0.10996900
H	0.66730400	4.76106900	-0.07871400
C	-1.30923200	3.80677500	-0.21655500
H	-2.06621800	4.56875100	-0.28055400
C	1.91820500	2.17530300	0.09194000
H	2.16575100	1.66957400	-0.84801700
C	2.02567900	1.08538900	1.19244500
C	2.87712500	3.36334200	0.24167000
H	2.60497000	4.06752900	-0.55707200
C	-2.98880200	2.01038400	-0.19460500
C	-3.69219000	1.88626400	-1.39426100
C	-3.58933700	1.80780800	1.04998900
C	-5.03854500	1.54104100	-1.31740300
C	-4.93925900	1.46661100	1.07140900
C	-5.67893700	1.32832400	-0.09982100
H	-5.59655400	1.42552600	-2.24058400
H	-5.42321100	1.30933200	2.03021600
C	-7.12510200	0.92485400	-0.05574600
H	-7.57606000	1.15936000	0.90995300
H	-7.70251000	1.42829700	-0.83353900
H	-7.23051200	-0.15224600	-0.21816500
C	-3.02191100	2.07643600	-2.72037700
H	-2.45384900	3.00880300	-2.76322400
H	-2.33091800	1.24809900	-2.89191800
H	-3.75773000	2.08433000	-3.52436300

C	-2.81476000	1.96310300	2.32758100
H	-1.96634400	1.27568800	2.36923100
H	-2.40915900	2.97332600	2.43115200
H	-3.45403000	1.76841000	3.18897200
C	2.95032200	-2.50467700	2.13862600
H	2.19197600	-1.77632800	2.43617500
H	2.47272500	-3.48488000	2.07046700
H	3.71145800	-2.54581800	2.91763100
C	6.81863500	-0.59913100	-0.44313500
H	7.53742900	-1.42419300	-0.43496300
H	7.00721800	-0.00660100	-1.33971500
H	7.02888400	0.02425500	0.42829200
C	2.53080600	-1.71976800	-2.83392900
H	1.61948600	-1.12171800	-2.75204600
H	3.11182800	-1.34241100	-3.67569800
H	2.21848500	-2.74029300	-3.07124500
C	-2.32989700	-3.58122200	1.81367800
H	-2.79751300	-4.50202300	1.44083800
H	-1.25121900	-3.76114900	1.81763100
C	-4.14999400	-2.20170400	0.71098600
H	-4.64926400	-3.10534200	0.34667300
H	-4.58975800	-1.93756800	1.67345500
H	-4.37167400	-1.39556400	0.01206000
C	2.77873700	4.08882600	1.58725100
H	3.25605700	3.49787000	2.36751100
H	3.26547200	5.06495200	1.53237200
H	1.74444500	4.25688100	1.89490000
C	4.31277500	2.91710400	-0.06817700
H	4.63375400	2.21708500	0.70573400
H	4.30935900	2.36116400	-1.01273500
C	5.30051000	4.07173800	-0.17935100
H	5.42361500	4.59635300	0.77044400
H	6.28647000	3.70825100	-0.47827600
H	4.97958400	4.80448000	-0.92666900
C	-2.77875900	-3.32665600	3.24809100
H	-3.86451600	-3.25184200	3.33403500
H	-2.45501900	-4.13828300	3.90365000
H	-2.34699700	-2.39917900	3.63451800

Phe$_2$Ni

Ni	0.05144600	0.33251300	0.04334800
O	-1.12404300	-0.15629000	1.40326900
O	-2.91403400	0.00702000	2.69956600
N	0.43836800	3.29884200	0.42639700
N	-1.53302100	2.57928100	0.84065800
C	-0.31571500	2.17415100	0.43075000
C	-1.55881500	3.93729100	1.07878800
H	-2.44535600	4.45050300	1.40889900
C	-0.31145600	4.39152300	0.82301000
H	0.11516500	5.37652500	0.89743400
C	-2.66554700	1.67508500	1.02578200
H	-3.37171600	2.19642200	1.67081500
C	-2.20903600	0.41382200	1.79143100
C	-3.34298400	1.34005800	-0.31967800
H	-3.07396000	2.11996000	-1.03635200
H	-2.91647700	0.40920900	-0.71007900
C	1.85615300	3.37006100	0.20707000
C	2.70303000	3.08945000	1.28033000
C	2.33739600	3.75310000	-1.04696400
C	4.07647600	3.19687100	1.06744200
C	3.71527700	3.85244900	-1.20463800
C	4.59974400	3.57749200	-0.16442700
H	4.75098700	2.98171600	1.89025000
H	4.10664900	4.12733100	-2.17835600
O	1.20469200	0.80340500	-1.34089000
O	3.04975900	0.61731400	-2.55733100
N	-0.23792100	-2.64472300	-0.40853900
N	1.74849700	-1.86527200	-0.59722400
C	0.47960800	-1.50493100	-0.31459100
C	1.83523600	-3.21662500	-0.86250700
H	2.76234800	-3.71461100	-1.07947800
C	0.58102000	-3.70752600	-0.74611400
H	0.19676800	-4.70490700	-0.86931400
C	2.81775500	-0.85990000	-0.67944000

H	2.90607000	-0.41205200	0.31439900
C	2.34260100	0.27389100	-1.62914900
C	4.15568300	-1.43154300	-1.11226800
H	4.05063000	-1.89175800	-2.09792600
H	4.80087700	-0.56570100	-1.28127400
C	-1.66731400	-2.75754600	-0.33207300
C	-2.26217500	-3.15618500	0.86433700
C	-2.40745100	-2.51339800	-1.49360400
C	-3.64749700	-3.30968000	0.87364800
C	-3.78720600	-2.67635700	-1.42896000
C	-4.42490900	-3.07487700	-0.25510800
H	-4.12853800	-3.60898700	1.79877700
H	-4.37827500	-2.49012700	-2.32014100
C	-5.91882900	-3.21929800	-0.21126900
H	-6.29532100	-3.72339000	-1.10422700
H	-6.23708200	-3.79024100	0.66217800
H	-6.39784300	-2.23722700	-0.16146800
C	-1.45756100	-3.36685400	2.11071500
H	-0.56963300	-3.97652900	1.92928200
H	-1.13055300	-2.39729500	2.49414400
H	-2.05931500	-3.85401100	2.87799800
C	-1.74002600	-2.09362100	-2.77247000
H	-1.19807000	-1.15169200	-2.65432900
H	-1.01189600	-2.83702500	-3.10816600
H	-2.47812500	-1.96497400	-3.56438100
C	1.41144500	3.98459500	-2.20187300
H	0.98386100	3.02815700	-2.51254800
H	0.58967900	4.65678000	-1.94424400
H	1.95135800	4.41005200	-3.04760600
C	6.08260900	3.68185100	-0.37978800
H	6.36895200	4.69821800	-0.66311700
H	6.63662900	3.41631100	0.52157100
H	6.40716000	3.01747800	-1.18483400
C	2.16235700	2.68275300	2.62163300
H	1.59586400	1.74972000	2.56159200
H	2.97446500	2.54308600	3.33550500
H	1.48431100	3.43807300	3.02784800
C	-4.84839200	1.23218500	-0.26899900
C	-5.59795700	1.66217100	-1.36545400
C	-5.52305100	0.70690000	0.83468600
C	-6.98416500	1.57005400	-1.36716500
H	-5.08869700	2.07880600	-2.22888500
C	-6.91153600	0.62417300	0.83686700
H	-4.96180200	0.36128400	1.69670200
C	-7.64774200	1.05148100	-0.26157500
H	-7.54560400	1.91262100	-2.22899300
H	-7.41893900	0.22086100	1.70612700
H	-8.72960400	0.98561200	-0.25485000
C	4.83070000	-2.38903000	-0.15870600
C	5.53020500	-3.48560100	-0.66606300
C	4.82499600	-2.19763900	1.22365900
C	6.20034500	-4.36520400	0.17562900
H	5.55440800	-3.64837800	-1.73925200
C	5.49135300	-3.07581900	2.06960400
H	4.29800900	-1.35355800	1.65431900
C	6.18105400	-4.16457800	1.55005100
H	6.73679400	-5.20844300	-0.24415100
H	5.47022700	-2.90794300	3.14030100
H	6.69858200	-4.84988700	2.21080800