Supporting Information

for

Nickel(I)-mediated transformations of carbon dioxide in closed synthetic cycles: reductive cleavage and coupling of CO_2 generating $Ni^{I}CO$, $Ni^{II}CO_3$ and $Ni^{II}C_2O_4Ni^{II}$ entities

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General Procedures

All manipulations were carried out in a glove box, or else by means of Schlenk-type techniques involving the use of a dry argon atmosphere. Solvents were dried employing a MBraun Solvent Purification System SPS. The ^{1}H spectra were recorded on a Bruker DPX 300 NMR spectrometer (300.1 MHz) with dry benzene-d_6 or dmso-d_6 as solvent at 20 °C and calibrated against the residual proton resonances of the deuterated solvents (benzene-d_6: δ_H 7.16 ppm, dmso-d_6: δ_H 2.50 ppm). The ^{13}C NMR spectrum was recorded on a Bruker DPX 300 NMR spectrometer (75.5 MHz) with deuterium oxide as solvent at 20 °C. Solution magnetic susceptibilities were determined by the Evans method[S1] at room temperature with a Bruker DPX 300 NMR spectrometer (300.1 MHz). The samples were measured in thf-d_8 with 1 % tetramethylsilane (TMS), together with a capillary tube that contained thf-d_8 with 1 % TMS as an internal standard. For the diamagnetic correction of the susceptibility, Pascal's constants[S2] were used. Infrared (IR) spectra were recorded using solid samples prepared as KBr pellets with a Shimadzu FTIR-8400S-spectrometer. Microanalyses were performed on a HEKAtech Euro EA 3000 analyser. EPR spectra were recorded at the X-band spectrometer *ERS 300* equipped with a fused quartz Dewar for measurements at liquid nitrogen temperature. The *g*-factors were calculated with respect to a Cr^{3+}/MgO reference (g = 1.9796).

Experimental Section – Spectroscopic Details

Reaction of $K_2[L^{tBu}Ni(N_2)NiL^{tBu}]$[S3], I, with CO_2. A dark purple suspension of $K_2[L^{tBu}Ni(N_2)NiL^{tBu}]$[S3], **I**, (42 mg, 0.03 mmol) in hexane was exposed to a CO_2 atmosphere. Subsequently, a colour change and formation of a golden brown solution was observed. The reaction mixture was stirred at room temperature for 18 h. All volatiles were removed in vacuum to give a golden brown residue, which was characterised by IR, ^{1}H NMR, and EPR spectroscopy. The IR spectrum of the crude product and a ^{1}H NMR spectrum of a benzene-d_6 solution indicated the presence of **II**[S4] and **III**[S5] (see Figures S1-S3), respectively. An EPR spectrum of a hexane solution of the crude product (see Figure S4) indicated the presence of a nickel(I) species, consistent with the formation of **II**[S4] (reference spectrum see Figure S5) during the course of the reaction.

Isolation of III[S5]: reaction of $K_2[L^{tBu}Ni(N_2)NiL^{tBu}]$[S3], I, with CO_2. A dark purple suspension of $K_2[L^{tBu}Ni(N_2)NiL^{tBu}]$[S3], **I**, (47 mg, 0.04 mmol) in hexane was exposed to a CO_2 atmosphere. Subsequently, a colour change and formation of a golden brown solution was observed. The reaction mixture was stirred at room temperature for 18 h. All volatiles were removed in vacuum. The remaining light brown residue was extracted with 3 mL hexane and the resulting solution was cooled to -30 °C for 1 day. Filtration and drying of the remaining residue in vacuum yielded a light brown solid of $K_6[L^{tBu}Ni(CO_3)]_6$[S5], **III** (18 mg, 4.6 µmol, 36 %). ^{1}H NMR (300.1 MHz, dmso-d_6): δ = 6.83 (m, $^3J_{HH}$ = 7.5 Hz, 2H, Ar-*pH*), 6.72 (m, $^3J_{HH}$ = 7.2 Hz, 4H, Ar-*mH*), 4.98 (s, 1H, C*H*CC(CH$_3$)$_3$), 3.90 (m, $^3J_{HH}$ = 6.8 Hz, 4H, C*H*(CH$_3$)$_2$), 1.74 (d, $^3J_{HH}$ = 6.6 Hz, 12H, CH(C*H*$_3$)$_2$), 1.27 (d, $^3J_{HH}$ = 6.6 Hz, 12H, CH(C*H*$_3$)$_2$), 0.84 (s, 18H, C(C*H*$_3$)$_3$) ppm; ^{1}H NMR (300.1 MHz, C_6D_6): δ = 7.11-6.80 (br, 6H, Ar-*H*), 5.39 (s, 1H, C*H*CC(CH$_3$)$_3$), 4.23 (br, 4H, C*H*(CH$_3$)$_2$), 2.29-1.89 (br, 12H, CH(C*H*$_3$)$_2$), 1.54-1.27 (br, 12H, CH(C*H*$_3$)$_2$), 1.07 (br, 18H, C(C*H*$_3$)$_3$) ppm; IR (KBr): υ = 3055 (w), 3017 (m), 2960 (vs), 2930 (s), 2908 (s), 2869 (s), 1615 (vs), 1597 (vs), 1533 (m), 1519 (s), 1464 (m), 1445 (m), 1435 (m), 1408 (vs), 1383 (m), 1368 (s), 1322 (vs), 1252 (w), 1219 (m), 1207 (w), 1192 (w), 1183 (w), 1164 (m), 1149 (w), 1098 (m), 1056 (m), 1030 (m), 976 (w), 934 (w), 835 (w), 806 (m), 784 (m), 765 (m), 729 (w), 718 (w), 683 (w) cm^{-1}.

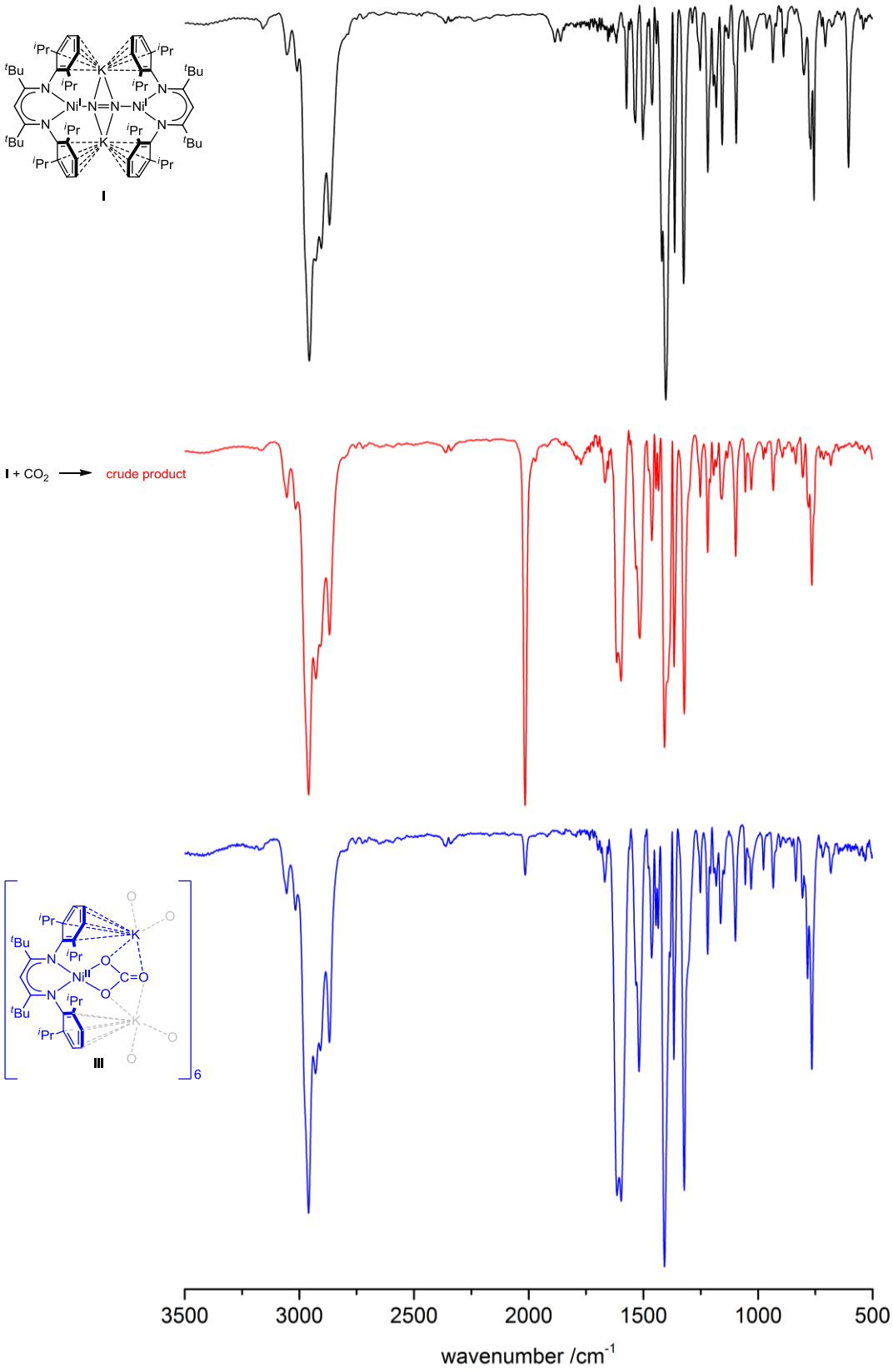


Figure S1. IR spectra (KBr) of $K_2[L^{tBu}Ni(N_2)NiL^{tBu}]$[S3], **I** (black line, top), the crude product from the reaction of **I**[S3] with CO_2 (red line, middle), and isolated $K_6[L^{tBu}NiCO_3]_6$[S5], **III** (blue line, bottom).

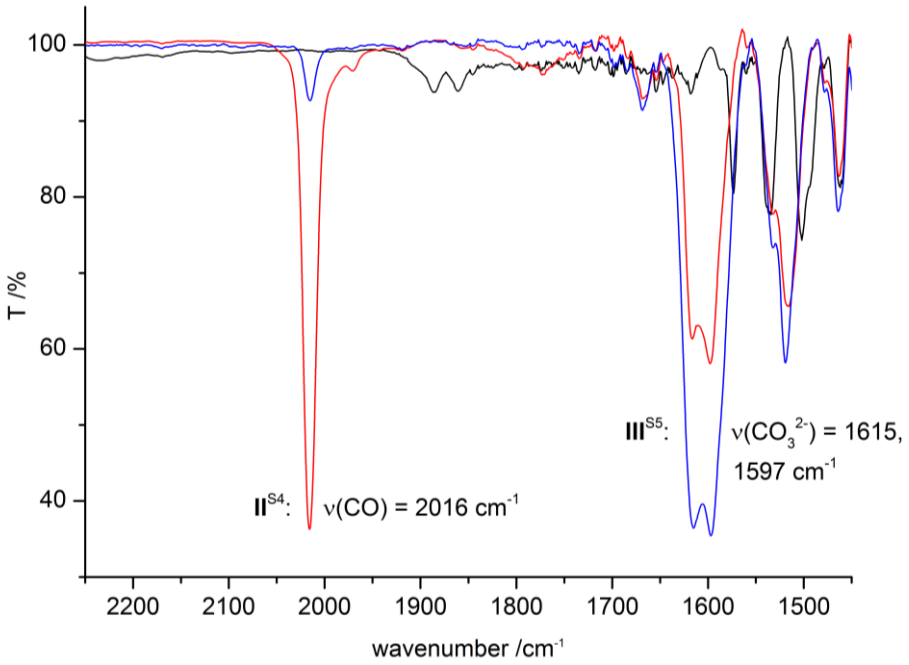


Figure S2. ν_{CO} region of the IR spectra (KBr) recorded for $K_2[L^{tBu}Ni(N_2)NiL^{tBu}]$[S3], **I** (black line), the crude product from the reaction of **I**[S3] with CO_2 (red line), and isolated $K_6[L^{tBu}NiCO_3]_6$[S5], **III** (blue line).

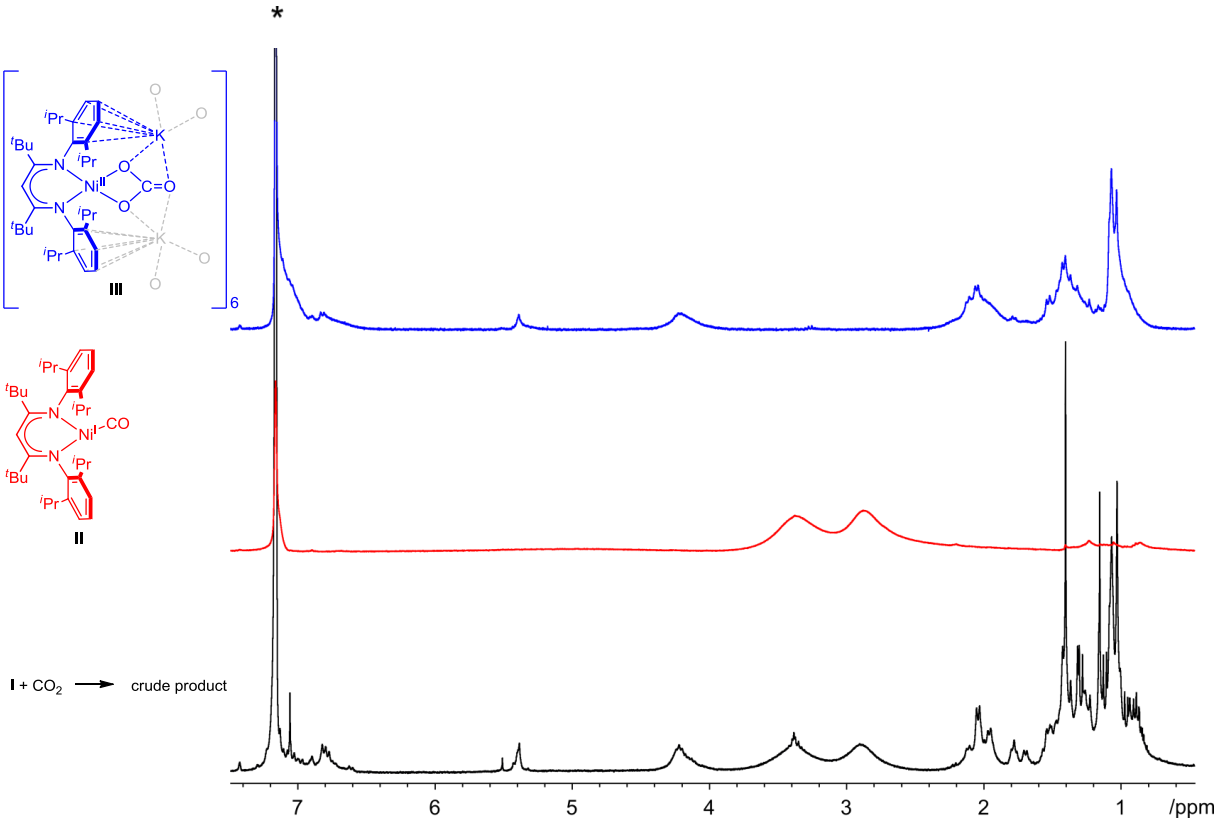


Figure S3. ^{1}H NMR spectra of the crude product from the reaction of **I**[S3] with CO_2 (black line) and isolated $K_6[L^{tBu}NiCO_3]_6$[S5], **III** (blue line), and pure $[L^{tBu}NiCO]$[S4], **II** (red line) in benzene-d_6 (*).

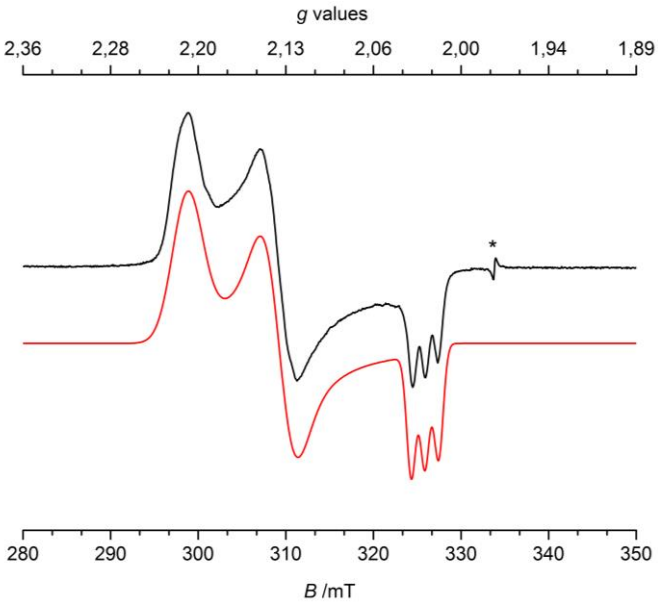


Figure S4. EPR spectrum after the reaction of **I**[S3] dissolved in hexane with CO_2 after 12 h; the sample was taken directly from the reaction mixture and cooled to 77 K. Black line: Experimental spectrum with MgO/Cr^{3+} (*) as an internal standard. Red line: Powder Simulation, the g values were determined to g_x = 2.216, g_y = 2.140, g_z = 2.031 (A_{zz} = 1.4 mT, spectrometer frequency: 9.246 GHz).

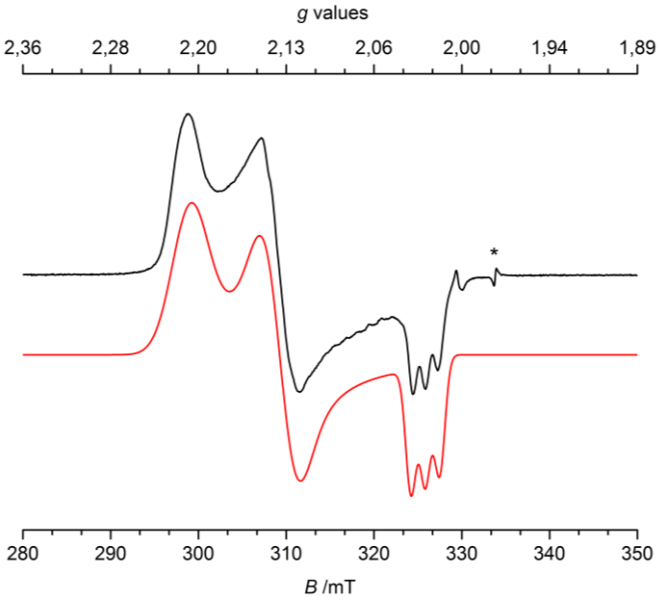


Figure S5. Reference EPR spectrum of a hexane solution of **II**[S4] recorded at 77 K. Black line: Experimental spectrum with MgO/Cr^{3+} (*) as an internal standard. Red line: Powder Simulation, the g values were determined to g_x = 2.215, g_y = 2.140, g_z = 2.031 (A_{zz} = 1.4 mT, spectrometer frequency: 9.246 GHz).

Reaction of $K_2[L^{tBu}Ni(CO)]_2$[S4] with CO_2. An orange suspension of $K_2[L^{tBu}Ni(CO)]_2$[S4] (20 mg, 0.02 mmol) in hexane was exposed to a CO_2 atmosphere. The reaction mixture was stirred at room temperature for 30 minutes. Afterwards, all volatiles were removed in vacuum to give a dark brown residue, which according to analysis by IR and ^{1}H NMR spectroscopy represented a mixture of diverse products including **II**[S4] and **III**[S5].

Reaction of $K_6[L^{tBu}Ni(CO_3)]_6$[S5], III, with KC_8 and N_2. $K_6[L^{tBu}Ni(CO_3)]_6$[S5], **III**, (96 mg, 24.3 µmol) and KC_8 (70 mg, 0.52 mmol) were suspended in hexane, and the reaction mixture was stirred for 48 h in a dinitrogen atmosphere at room temperature. Filtration of the resulting dark purple suspension* and removal of the solvent from the filtrate afforded **I**[S3] (61 mg, 0.05 mmol, 68 %) as a dark purple solid. ^{1}H NMR (300.1 MHz, C_6D_6): δ = 6.77 (s, 12H, Ar-*H*), 5.06 (s, 2H, C*H*C(CH$_3$)$_3$), 3.72 (m, $^3J_{HH}$ = 6.8 Hz, 8H, C*H*(CH$_3$)$_2$), 1.50 (d, $^3J_{HH}$ = 6.6 Hz, 24H, CH(C*H*$_3$)$_2$), 1.30 (d, $^3J_{HH}$ = 6.9 Hz, 24H, CH(C*H*$_3$)$_2$), 1.17 ppm (s, 36H, C(C*H*$_3$)$_3$) ppm.

*^{13}C NMR spectroscopy of a deuterium oxide solution of the remaining black residue proved the formation of K_2CO_3 during the course of the reduction of **III**[S5] with KC_8. ^{13}C{^{1}H} NMR (75.5 MHz, D_2O): δ = 168.3 (K_2CO_3) ppm.

Reaction of [L^{tBu}Ni(N$_2$)NiL^{tBu}]^{S3}, IV, with CO$_2$. A red brown hexane suspension of [L^{tBu}Ni(N$_2$)NiL^{tBu}]^{S3}, **IV**, (100 mg, 0.09 mmol) was exposed to a CO_2 atmosphere and the reaction mixture was stirred at room temperature for 24 h to give a dark brown suspension. Afterwards, all volatiles were removed in vacuum to yield a brown violet residue. The crude product was analysed by ^{1}H NMR, IR and EPR spectroscopy. The ^{1}H NMR (C_6D_6) and IR (KBr) spectra showed the signal set of **1** (see Figures S6-S9). The EPR spectrum of the crude product dissolved in hexane (see Figure S10) indicated the presence of at least one nickel(I) species, that could correspond to either **II**^{S4} (reference spectrum see Figure S5) or **IV**^{S3} (reference spectrum see Figure S11).

Isolation of 1: reaction of [L^{tBu}Ni(N$_2$)NiL^{tBu}]^{S3}, IV, with CO$_2$. A red brown hexane suspension of [L^{tBu}Ni(N$_2$)NiL^{tBu}]^{S3}, **IV**, (100 mg, 0.09 mmol) was exposed to a CO_2 atmosphere and the reaction mixture was stirred at room temperature for 60 h to give a dark brown suspension. All volatiles were removed in vacuum and the remaining brown violet residue was extracted with 3 mL hexane and cooled to -30 °C for 2 days. Filtration and drying of the remaining residue in vacuum yielded **1** (21 mg, 0.02 mmol, 20 %) as a violet solid.

Alternative synthesis of [L^{tBu}Ni(C$_2$O$_4$)NiL^{tBu}], 1. [L^{tBu}NiBr]^{S3}, **V**, (100 mg, 0.16 mmol) and $(NBu_4)_2C_2O_4$ (60 mg, 0.11 mmol) were suspended in diethyl ether and refluxed at 65 °C for 12 h. All volatiles were removed in vacuum and the remaining violet brown residue was washed with acetonitrile and dried in vacuum to give **1** (56 mg, 0.05 mmol) as a violet solid in 59 % yield. ^{1}H NMR (C_6D_6, 300.1 MHz): δ = 33 (8H, Ar-*mH*), 21 (8H, C*H*(CH$_3$)$_2$), 5 (24H, CH(C*H*$_3$)$_2$), 4 (24H, CH(C*H*$_3$)$_2$), 1 (36H, C(C*H*$_3$)$_3$), -29 (4H, Ar-*pH*), -123 (2H, C*H*CC(CH$_3$)$_3$) ppm; μ_{eff} (thf-d_8, 300.1 MHz) = 3.96 μ_B, IR (KBr): υ = 3056 (w), 3023 (w), 2960 (s), 2929 (m), 2907 (m), 2869 (m), 1652 (vs), 1649 (vs), 1619 (w), 1540 (m), 1508 (m), 1464 (m), 1459 (m), 1446 (w), 1432 (m), 1400 (m), 1383 (m), 1380 (m), 1363 (s), 1315 (m), 1252 (m), 1219 (w), 1204 (w), 1193 (w), 1179 (w), 1155 (w), 1133 (w), 1100 (m), 1055 (w), 1027 (w), 933 (w), 843 (w), 799 (m), 779 (m), 768 (m), 754 (m), 679 (w) cm^{-1}; Elemental analysis calc. (%) for $C_{72}H_{106}N_4Ni_2O_4$ (1209.02 g·mol^{-1}): C 71.53, H 8.84, N 4.63; found: C 71.13, H 8.87, N 4.64. Crystals suitable for X-ray diffraction analysis were grown from a benzene-d_6 solution.

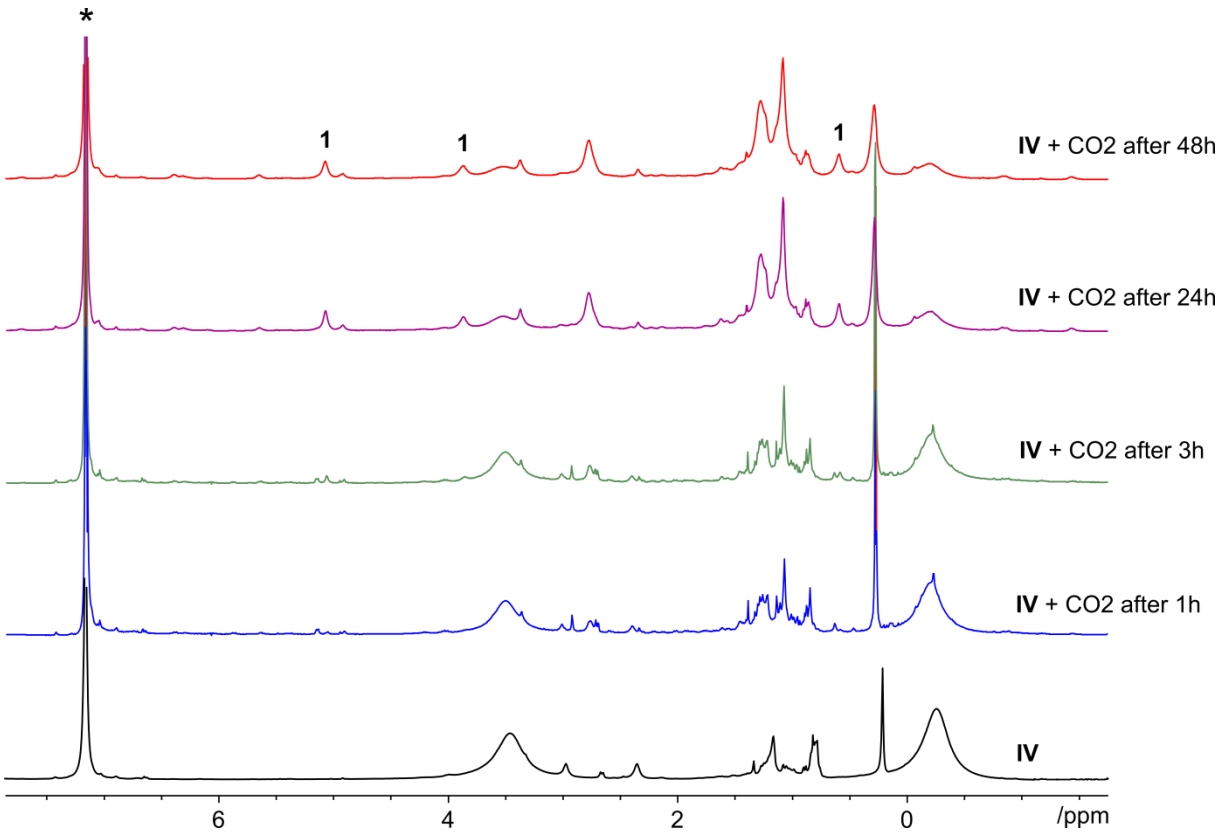


Figure S6. Reaction of [L^{tBu}Ni(N$_2$)NiL^{tBu}][S3], **IV**, with CO_2 in benzene-d_6 (*) under formation of **1** monitored by ^{1}H NMR spectroscopy over a period of 48h.

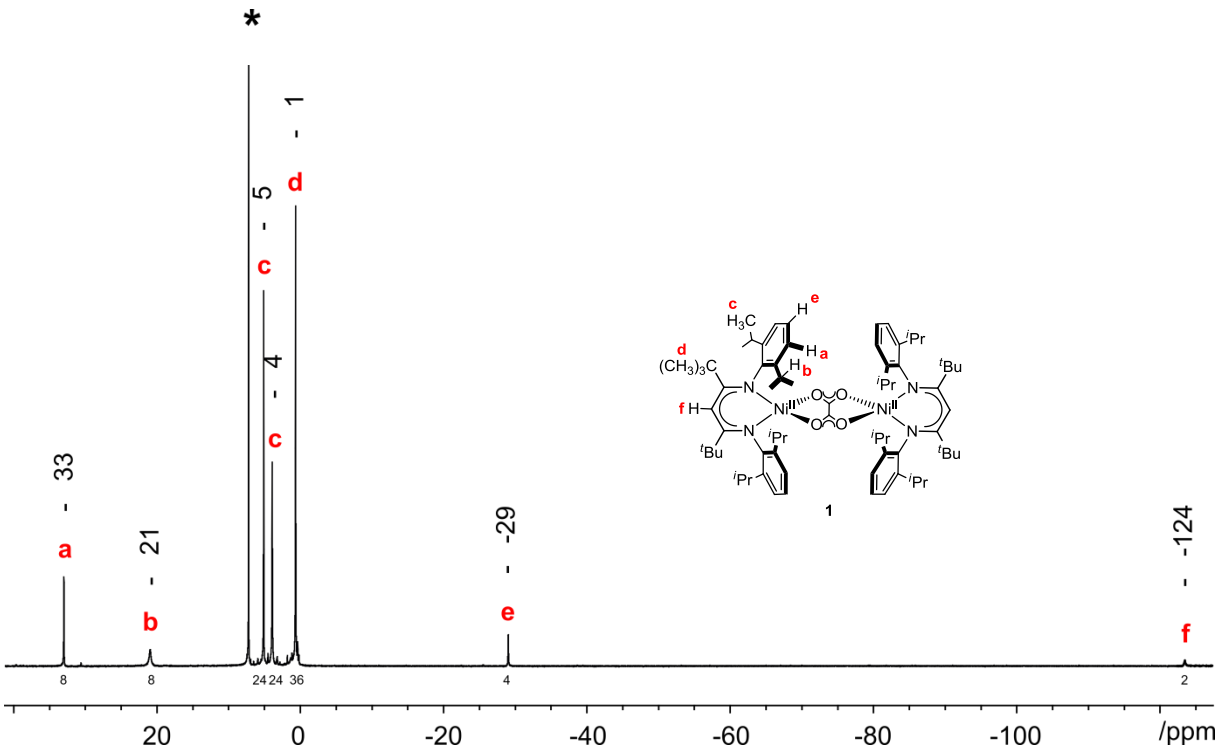


Figure S7. ^{1}H NMR spectrum of purified [L^{tBu}Ni(C$_2$O$_4$)NiL^{tBu}], **1**, dissolved in benzene-d_6 (*).

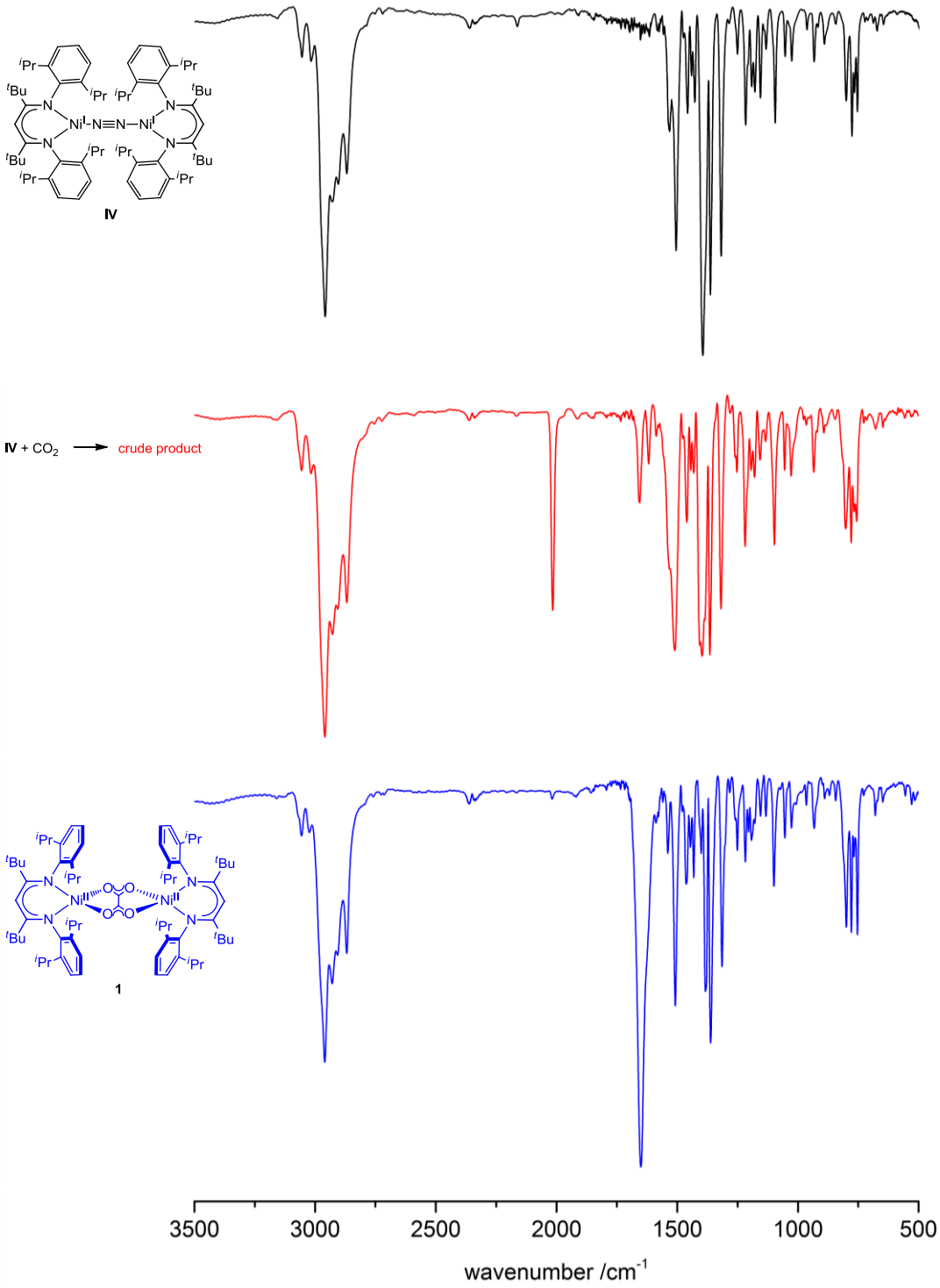


Figure S8. IR spectra (KBr) of [$L^{tBu}Ni(N_2)NiL^{tBu}$][S3], **IV** (black line, top), the crude product from the reaction of **IV**[S3] with CO_2 (red line, middle), and isolated [$L^{tBu}Ni(C_2O_4)NiL^{tBu}$], **1** (blue line, bottom).

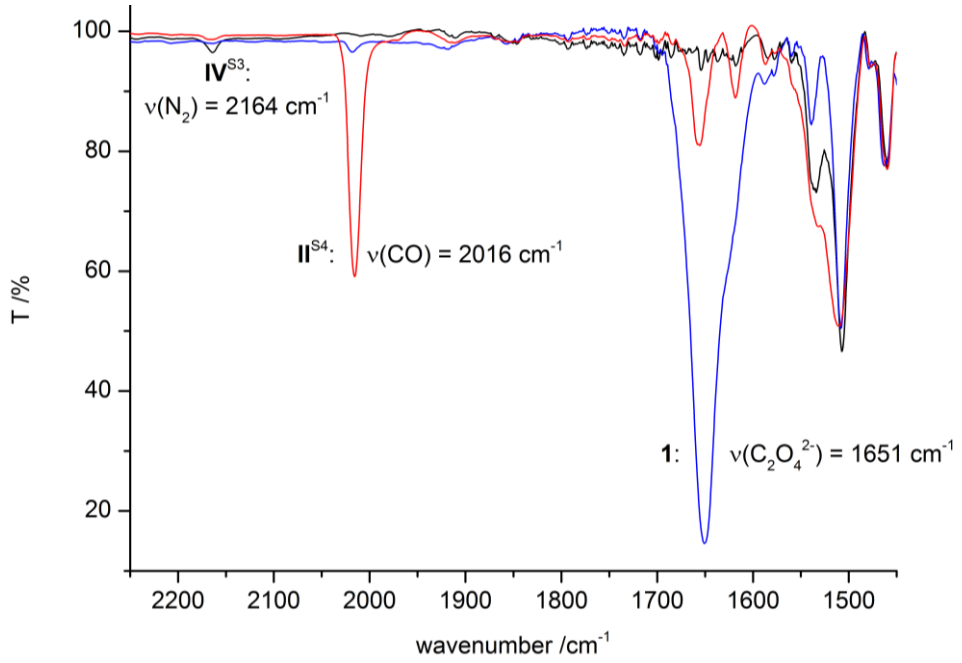


Figure S9. ν_{CO} regions of the IR spectra (KBr) recorded for [L$^{t\mathrm{Bu}}$Ni(N$_2$)NiL$^{t\mathrm{Bu}}$]^{S3}, **IV** (black line), the crude product from the reaction of **IV**^{S3} with CO_2 (red line), and isolated [L$^{t\mathrm{Bu}}$Ni(C$_2$O$_4$)NiL$^{t\mathrm{Bu}}$], **1** (blue line).

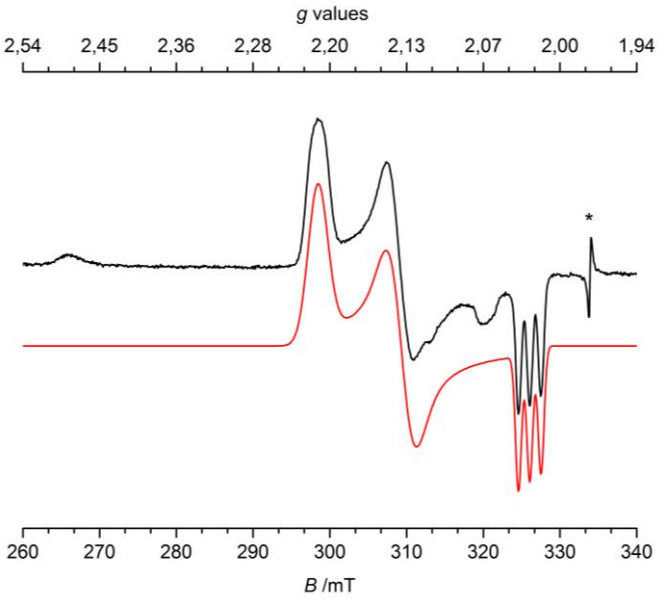


Figure S10. EPR spectrum after the reaction of **IV**^{S3} dissolved in hexane with CO_2 after 18 h; the sample was directly taken from the reaction mixture and cooled to 77 K. Black line: Experimental spectrum with MgO/Cr^{3+} (*) as an internal standard. Red line: Powder Simulation, the g values were determined to g_x = 2.214, g_y = 2.136, g_z = 2.027 (A_{zz} = 1.4 mT, spectrometer frequency: 9.246 GHz).

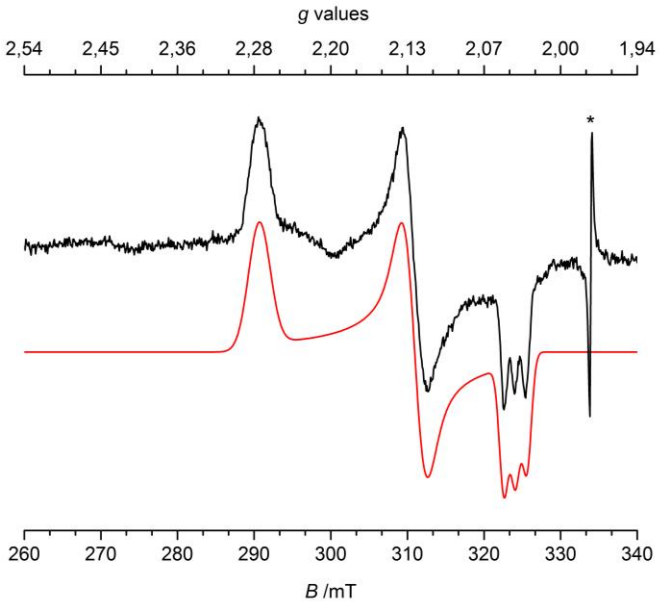


Figure S11. Reference EPR spectrum of a hexane solution of **IV**^{S3} recorded at 77 K. Black line: Experimental spectrum with MgO/Cr^{3+} (*) as an internal standard. Red line: Powder Simulation, the *g* values were determined to g_x = 2.273, g_y = 2.125, g_z = 2.039 (A_{zz} = 1.4 mT, spectrometer frequency: 9.246 GHz).

Reaction of [L^{tBu}Ni(C$_2$O$_4$)NiL^{tBu}], 1, with KC$_8$. [L^{tBu}Ni(C$_2$O$_4$)NiL^{tBu}], **1**, (16 mg, 13.2 µmol) and KC_8 (3.8 mg, 28.1 µmol) were suspended in hexane, and the reaction mixture was stirred for 12 h in a dinitrogen atmosphere. Filtration of the red brown suspension and removal of the solvent afforded a red brown solid of **IV**^{S3} (14 mg, 12.2 µmol, 92 %), as revealed by a ^{1}H NMR spectrum of a benzene-d_6 solution featuring two broad signals, which are characteristic for the nickel(I) dinitrogen compound, **IV**^{S3}: ^{1}H NMR (C_6D_6, 300.1 MHz): δ = 3.5 (br), -0.2 (br) ppm; IR (KBr): υ = 2164 (w, N_2) cm^{-1}.

X-Ray Crystallographic Data

Crystal data for **1**·4C_6D_6: $C_{96}H_{106}D_{24}N_4Ni_2O_4$, M = 1545.26 g·mol^{-1}, monoclinic, space group P 2_1/c, Z = 2, a = 17.3703(7) Å, b = 22.7046(6) Å, c = 10.8435(4) Å, α = 90°, β = 95.275(3)°, γ = 90°, V = 4258.4(3) Å^3, ρ_{calcd} = 1.205 g·cm^{-3}, T = 183(2) K, F_{000} = 1644, μ = 0.495 mm^{-1}, θ = 2.35-26.84°, reflections collected 30295, unique reflections 8989 [R_{int} = 0.0480], GoF = 1.004, R_1 = 0.0316 [$I > 2\sigma(I)$] and wR_2 = 0.0667, largest difference peak and hole 0.276/-0.394 e Å^{-3}. Crystallographic data were collected on a STOE IPDS 2T diffractometer (Mo-K_α radiation, λ = 0.71073 Å). The structure was solved by direct methods (SHELXS-97)[S6] and refined by full-matrix least-squares procedures based on F^2 with all measured reflections (SHELXL-97)[S7]. Multi-Scan (PLATON)[S8] absorption correction have been applied. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were added geometrically and refined by using a riding model. CCDC 950231 (**1**·4C_6D_6) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

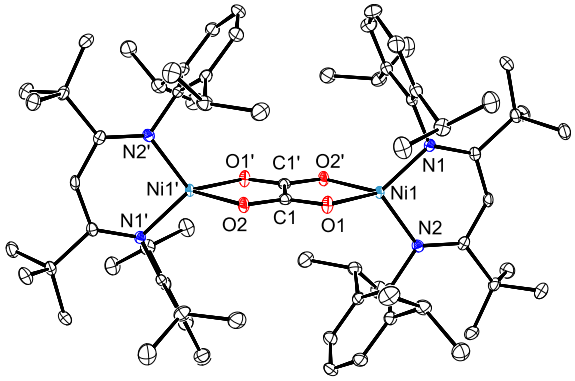


Figure S12. Molecular structure of **1**·4C_6D_6. Thermal ellipsoids are shown at 50% probability. Four co-crystallised benzene solvent molecules and the carbon bound hydrogen atoms are omitted for clarity. Selected bond lengths /Å and angles /°: Ni1–N1 1.9008(11), Ni1–N2 1.9111(11), Ni1–O2' 1.9927(10), Ni1–O1 2.0073(10), O1–C1 1.2553(16), O2–C1 1.2534(16), C1–C1' 1.527(3), N1-Ni1-N2 97.71(5), N1-Ni1-O1 127.97(5), N1-Ni1-O2' 116.39(4), N2-Ni1-O1 116.22(5), N2-Ni1-O2' 116.82(5), O2'-Ni1-O1 83.20(4), C1-O1-Ni1 111.33(9), C1-O2-Ni1' 111.96(9), O2-C1-O1 126.52(13), O2-C1-C1' 116.66(14), O1-C1-C1' 116.81(14).

Density Functional Calculations

Geometry optimizations were performed in redundant internal coordinates using the Gaussian09 program package.[S9] Molecular structures as determined by X-ray diffraction analysis were used as starting geometries wherever possible. The B3LYP functional[S10] was employed together with the 3-21G basis set for C and H atoms and the 6-31G* basis set for Ni, N, and O atoms, as implemented in Gaussian. Very tight convergence criteria were chosen for the SCF procedure and a pruned (99,590) "ultrafine" integration grid was used for numerical integrations. A search for broken symmetry solutions was performed (where appropriate) utilizing the fragment guess utility of the Gaussian09 program package.

Vibrational frequencies were computed analytically by determining the second derivatives of the energy with respect to the Cartesian nuclear coordinates and then transforming to mass-weighted coordinates. Reaction energies were calculated using electronic energies corrected by zero-point vibrational energies.

For the mononuclear Ni-CO_2 complexes, that required a Natural Bond Orbital (NBO) analysis, a further optimization using the Def2-SVP basis set[S11] for C and H atoms and the Def2-TZVPD basis set[S12] for Ni, N, and O atoms was performed. Both basis sets were taken from the EMSL Basis Set Exchange Database[S13]. Subsequently, the program NBO5.9[S14] was used for NBO analysis. Visualization of molecular structures was accomplished with the program GaussView5.

A) Detailed analysis of neutral and anionic mononuclear Ni-CO_2 complexes [L$^{t\mathrm{Bu}}$Ni(CO_2)] and [L$^{t\mathrm{Bu}}$Ni(CO_2)]$^-$ (B3LYP/Def2-SVP/TZVP):

The optimized structures of [L$^{t\mathrm{Bu}}$Ni(CO_2)] and [L$^{t\mathrm{Bu}}$Ni(CO_2)]$^-$ are shown in Figure S13 (basis set Def2-SVP/TZVP), NBO charges are displayed in Table S1.

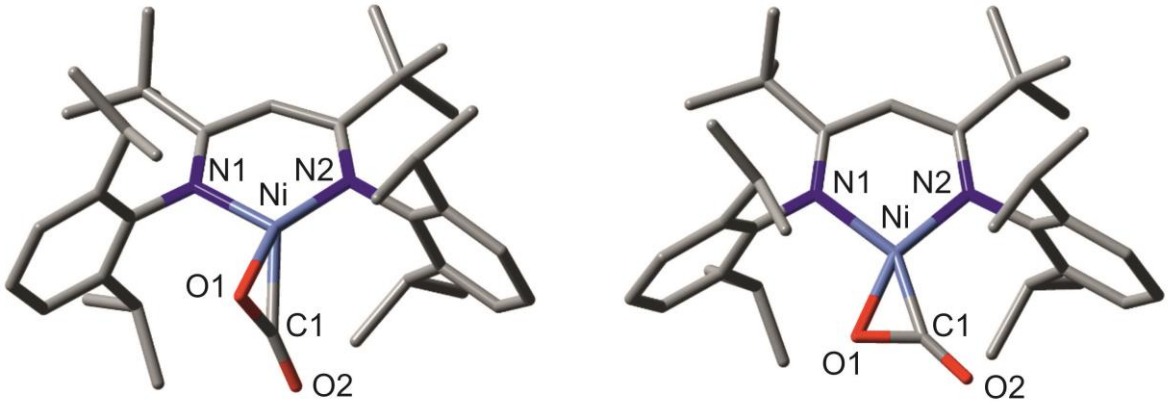


Figure S13. Optimized molecular structures for the ground states of [L^{tBu}Ni(CO$_2$)] and [L^{tBu}Ni(CO$_2$)]$^-$ (Def2-SVP/TZVP). Hydrogen atoms are omitted for clarity.

[L^{tBu}Ni(CO$_2$)] (neutral)		**[L^{tBu}Ni(CO$_2$)]$^-$ (anionic)**	
Ni	+0.91	Ni	+0.63
C1	+0.91	C1	+0.64
O1	-0.54	O1	-0.75
O2	-0.63	O2	-0.71
L^{tBu}	-0.65	L^{tBu}	-0.81

Table S1. NBO charges for selected atoms of [L^{tBu}Ni(CO$_2$)] and [L^{tBu}Ni(CO$_2$)]$^-$ (ground states, Def2-SVP/TZVP).

For the neutral [L^{tBu}Ni(CO$_2$)] a doublet ground state is found with a mulliken atomic spin density of 0.91 at the Ni atom. According to NBO analysis the Ni has a d^9 configuration corresponding to Ni^I, with no bonds to neighbouring atoms. Assigning integer charges to the molecular fragments gives the formula [(L^{tBu})$^-$(Ni)$^+$(CO$_2$)^0].

The [L^{tBu}Ni(CO$_2$)]$^-$ anion has a singlet ground state (the triplet state lies 70 kJ/mol higher in energy). NBO analysis finds one covalent Ni–C1 bond and 8 electrons in d-orbitals of the Ni atom. Applying formal heterolytic bond scission, we find an oxidation state of +II for Ni. In the heterolytic picture the anion can be described as [(L^{tBu})$^-$(Ni)$^{2+}$(CO$_2$)$^{2-}$]$^-$, however the alternative characterisation as [(L^{tBu})$^-$(Ni)$^+$–(CO$_2$)$^-$]$^-$ including the covalent Ni–C bond seems to be more appropriate.

B) Reaction energies (B3LYP/3-21G/6-31G*):

neutral complexes:

2 [L$^{t\mathrm{Bu}}$Ni(CO$_2$)] doublet (-3164.283043) -3163.453584	+	[L$^{t\mathrm{Bu}}$Ni(N$_2$)NiL$^{t\mathrm{Bu}}$] triplet (-6061.400344) -6059.757791	→	2 [L$^{t\mathrm{Bu}}$Ni(CO$_2$)NiL$^{t\mathrm{Bu}}$] triplet (-6140.235883) -6138.586284	+	N$_2$ singlet (-109.524129) -109.518530		-68.6 kJ/mol
2 [L$^{t\mathrm{Bu}}$Ni(CO$_2$)] doublet (-3164.283043) -3163.453584			→	[L$^{t\mathrm{Bu}}$Ni(C$_2$O$_4$)NiL$^{t\mathrm{Bu}}$] quintet (-6328.672432) -6327.010462				-271.2 kJ/mol
2 CO$_2$ singlet (-188.363023) -188.351391	+	[L$^{t\mathrm{Bu}}$Ni(N$_2$)NiL$^{t\mathrm{Bu}}$] triplet (-6061.400344) -6059.757791	→	2 [L$^{t\mathrm{Bu}}$Ni(CO$_2$)] doublet (-3164.283043) -3163.453584	+	N$_2$ singlet (-109.524129) -109.518530		+91.6 kJ/mol
CO$_2$ singlet (-188.363023) -188.351391	+	[L$^{t\mathrm{Bu}}$Ni(N$_2$)NiL$^{t\mathrm{Bu}}$] triplet (-6061.400344) -6059.757791	→	[L$^{t\mathrm{Bu}}$Ni(CO$_2$)NiL$^{t\mathrm{Bu}}$] triplet (-6140.235883) -6138.586284	+	N$_2$ singlet (-109.524129) -109.518530		+11.5 kJ/mol
2 CO$_2$ singlet (-188.363023) -188.351391	+	[L$^{t\mathrm{Bu}}$Ni(N$_2$)NiL$^{t\mathrm{Bu}}$] triplet (-6061.400344) -6059.757791	→	[L$^{t\mathrm{Bu}}$Ni(C$_2$O$_4$)NiL$^{t\mathrm{Bu}}$] quintet (-6328.672432) -6327.010462	+	N$_2$ singlet (-109.524129) -109.518530		-179.6 kJ/mol
		[L$^{t\mathrm{Bu}}$Ni(N$_2$)NiL$^{t\mathrm{Bu}}$] triplet (-6061.400344) -6059.757791	→	[L$^{t\mathrm{Bu}}$Ni] doublet (-2975.898642) -2975.082512	+	[L$^{t\mathrm{Bu}}$Ni(N$_2$)] doublet (-3085.459008) -3084.634749		+106.4kJ/mol
		[L$^{t\mathrm{Bu}}$Ni(N$_2$)NiL$^{t\mathrm{Bu}}$] triplet (-6061.400344) -6059.757791	→	2 [L$^{t\mathrm{Bu}}$Ni] doublet (-2975.898642) -2975.082512	+	N$_2$ singlet (-109.524129) -109.518530		+194.9kJ/mol
N$_2$ singlet (-109.524129) -109.518530	+	[L$^{t\mathrm{Bu}}$Ni(N$_2$)NiL$^{t\mathrm{Bu}}$] triplet (-6061.400344) -6059.757791	→	2 [L$^{t\mathrm{Bu}}$Ni(N$_2$)] doublet (-3085.459008) -3084.634749				+17.9 kJ/mol
2 CO singlet (-113.094453) -113.089442	+	[L$^{t\mathrm{Bu}}$Ni(N$_2$)NiL$^{t\mathrm{Bu}}$] triplet (-6061.400344) -6059.757791	→	2 [L$^{t\mathrm{Bu}}$Ni(CO)] doublet (-3089.063578) -3088.239565	+	N$_2$ singlet (-109.524129) -109.518530		-160.1 kJ/mol

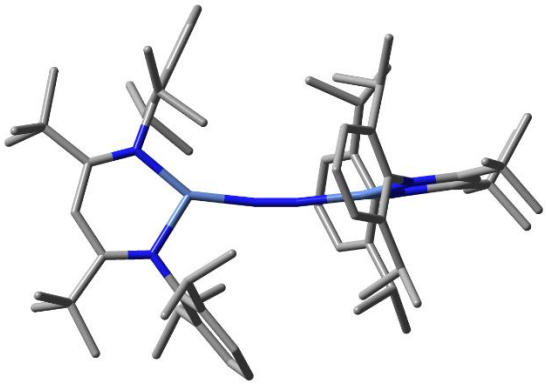
anionic complexes:

$[L^{tBu}Ni(CO_2)]^-$ singlet (-3164.340430) -3163.511886	→	$[L^{tBu}NiO]^-$ triplet (-3051.162043) -3050.344971	+	CO singlet (-113.094453) -113.089442	+203.4 kJ/mol
2 $[L^{tBu}Ni(CO_2)]^-$ singlet (-3164.340430) -3163.511886	→	$[L^{tBu}Ni(C(O)OC(O)O)NiL^{tBu}]^{2-}$ open-shell singlet (-6328.594051) -6326.940298			+219.2 kJ/mol
2 $[L^{tBu}Ni(CO_2)]^-$ singlet (-3164.340430) -3163.511886	→	$[L^{tBu}Ni(CO)(OC(O)O)NiL^{tBu}]^{2-}$ open-shell singlet (-6328.629754) -6326.975754			+126.1 kJ/mol

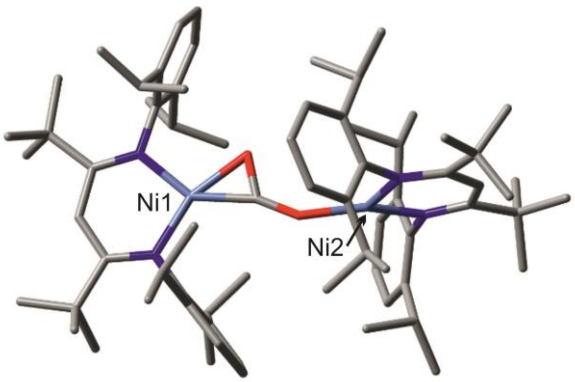
Table S2. Calculated reaction energies. For each reactant and product the ground state multiplicity, electronic energies (in brackets) and electronic energies corrected by zero-point vibrational energies are given (in hartree).

Table S2 summarises the set of reactions investigated. For each reactant and product a full geometry optimisation was performed followed by calculation of the vibrational frequencies. Below detailed information about geometric and electronic structure of the reactants and products are given.

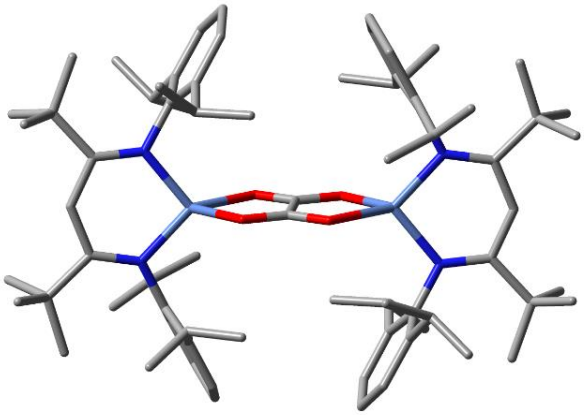
$[L^{tBu}Ni(N_2)NiL^{tBu}]$ has a triplet ground state with one unpaired electron at each Ni atom. The broken symmetry state with these two electrons coupled antiferromagnetically (open-shell singlet) is 5.9 kJ/mol higher in energy. The closed-shell singlet and the quintet state are 55.1 and 135.4 kJ/mol higher in energy than the triplet ground state, respectively.



[L$^{t\mathrm{Bu}}$Ni(CO$_2$)NiL$^{t\mathrm{Bu}}$] has a triplet ground state with two unpaired electrons at Ni2 and no unpaired electrons at Ni1 (cf. picture). The singlet and the quintet state are 31.6 and 10.5 kJ/mol higher in energy than the triplet ground state, respectively. According to an NBO analysis and restricting to integer charges of the molecular fragments the molecule should be described as [(L$^{t\mathrm{Bu}}$)$^-$(Ni)$^+$–(C(O)O)$^-$(Ni)$^{2+}$(L$^{t\mathrm{Bu}}$)$^-$] with one covalent Ni1-C bond. Assumption of formal heterolytic bond scission leads to the ionic description [(L$^{t\mathrm{Bu}}$)$^-$(Ni)$^{2+}$(C(O)O)$^{2-}$(Ni)$^{2+}$(L$^{t\mathrm{Bu}}$)$^-$] with one negative charge at each O atom.

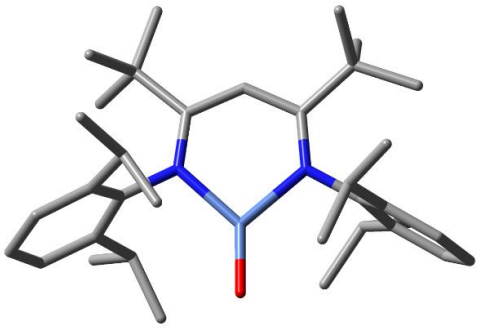


[L$^{t\mathrm{Bu}}$Ni(C$_2$O$_4$)NiL$^{t\mathrm{Bu}}$] has a quintet ground state with two unpaired electrons at each Ni atom. The broken symmetry state with these electrons coupled antiferromagnetically (open-shell singlet) is 79.4 kJ/mol higher in energy. The closed-shell singlet and the triplet states are 61.0 and 51.0 kJ/mol higher in energy than the quintet ground state, respectively.

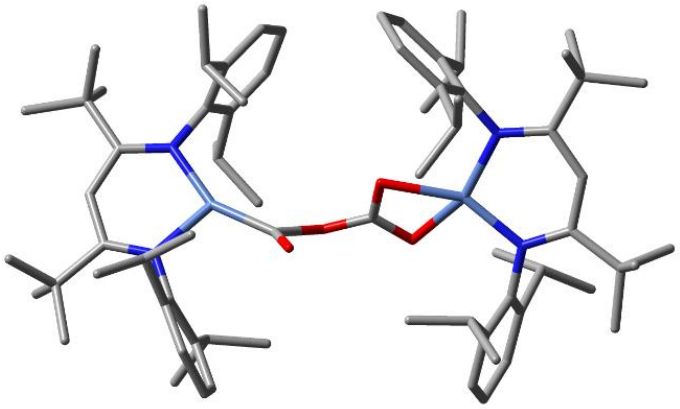


[L$^{t\mathrm{Bu}}$Ni], **[L$^{t\mathrm{Bu}}$Ni(N$_2$)]**, and **[L$^{t\mathrm{Bu}}$Ni(CO)]** have a doublet ground state each with one unpaired electron at the Ni atom.

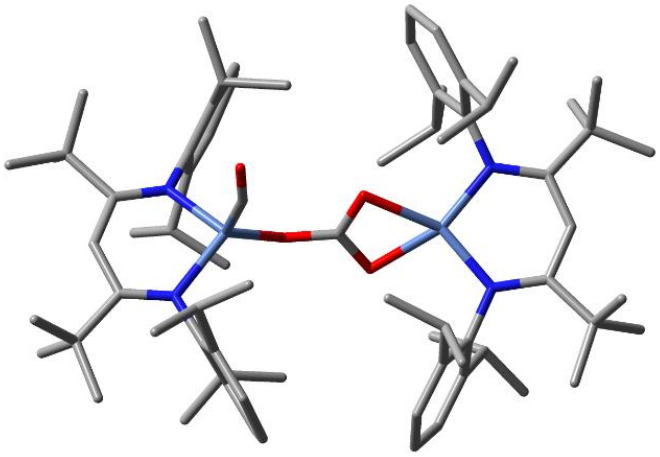
The **[L^{tBu}NiO]$^{-}$** anion has a triplet ground state with one unpaired electron each at the Ni and the O atom. No broken symmetry wave function with these two electrons coupled antiferromagnetically was found. The closed-shell singlet state is 57.0 kJ/mol higher in energy than the triplet ground state.



Several starting structures for the **[L^{tBu}Ni(C(O)OC(O)O)NiL^{tBu}]$^{2-}$** anion were optimised, resulting in the most favourable geometry shown here. This anion has an open-shell singlet ground state with one unpaired electron at each Ni atom, coupled antiferromagnetically. The corresponding triplet state, however, is only 46.4 J/mol higher in energy.



In the course of the optimisation of the [L^{tBu}Ni(C(O)OC(O)O)NiL^{tBu}]$^{2-}$ anion, also a structure of the anion **[L^{tBu}Ni(CO)(OC(O)O)NiL^{tBu}]$^{2-}$** was found. This anion has an open-shell singlet ground state, too, with one unpaired electron at each Ni atom, coupled antiferromagnetically. The corresponding triplet state is 252.4 J/mol higher in energy.



Cartesian coordinates (Å) for the theoretical structures obtained from geometry optimization (B3LYP/3-21G/6-31G*):

[L$^{t\text{Bu}}$Ni(CO_2)] (doublet state):

	x	y	z
Ni	0.075079	-0.844726	0.237869
H	0.805146	-1.022340	-2.629114
N	-1.462846	0.349269	0.035857
N	1.504687	0.404780	0.159490
C	1.634366	-0.732728	-3.285782
C	-1.299509	1.665462	0.054696
C	-2.686469	-0.391074	-0.005539
C	1.295972	1.727646	0.217588
C	2.727477	-0.317594	-0.026262
C	2.625598	0.199901	-2.567484
H	2.127251	-1.657251	-3.626038
H	1.207025	-0.228572	-4.168290
C	-0.007444	2.257166	0.153594
C	-2.450102	2.743255	0.004883
C	-3.203452	-0.837039	-1.252218
C	-3.290772	-0.803302	1.213593
C	2.462322	2.761775	0.450792
C	3.255096	-0.473557	-1.343956
C	3.309102	-1.028637	1.064173
H	2.043572	1.060390	-2.213448
C	3.662809	0.727781	-3.574444
H	-0.043983	3.332545	0.201435
C	-3.901040	2.227248	-0.064195
C	-2.234529	3.631356	-1.247518
C	-2.369513	3.622788	1.280273
C	-4.346219	-1.650215	-1.248427
C	-2.571361	-0.466329	-2.596644
C	-4.427694	-1.620147	1.155153
C	-2.741303	-0.401583	2.584358
C	1.951421	4.205303	0.664016
C	3.456712	2.827431	-0.728079
C	3.236312	2.379528	1.729979
C	4.361247	-1.313006	-1.526994
C	4.413253	-1.857780	0.814113
C	2.757614	-0.964236	2.491565
H	3.163492	1.342606	-4.340620
H	4.172576	-0.091308	-4.106737
H	4.435774	1.346648	-3.094900
H	-4.188407	1.640742	0.814622
H	-4.101813	1.617143	-0.949668
H	-4.569481	3.101941	-0.108841
H	-2.271845	3.031303	-2.169741
H	-1.271998	4.160152	-1.233924
H	-3.032542	4.389216	-1.307462
H	-3.191978	4.356245	1.274072
H	-1.428757	4.183270	1.360185
H	-2.473952	3.011414	2.190064
H	-4.762048	-1.989430	-2.200541
C	-4.963380	-2.038405	-0.061462
H	-1.662415	0.116780	-2.386548
C	-3.495857	0.407623	-3.466867
C	-2.149741	-1.712255	-3.398310
H	-4.904947	-1.938207	2.085562
H	-1.897748	0.283888	2.417650

C	-3.776827	0.345760	3.445483
C	-2.196901	-1.618958	3.356449
H	1.271842	4.288426	1.524645
H	1.443568	4.610564	-0.223694
H	2.816528	4.855923	0.864921
H	2.951948	3.094279	-1.668492
H	3.996680	1.885767	-0.873939
H	4.207709	3.607167	-0.522102
H	3.975907	3.162181	1.962803
H	3.782496	1.438897	1.608597
H	2.562516	2.285078	2.595477
H	4.773225	-1.440663	-2.529939
C	4.943194	-2.002452	-0.464113
H	4.866437	-2.405320	1.643847
H	2.016329	-0.152717	2.524020
C	2.034066	-2.269123	2.876982
C	3.838325	-0.653089	3.544210
H	-5.852794	-2.673061	-0.083928
H	-3.786054	1.341525	-2.965035
H	-4.422138	-0.128714	-3.730471
H	-2.991616	0.677670	-4.409161
H	-1.622408	-1.415898	-4.319279
H	-3.023746	-2.312606	-3.698409
H	-1.478013	-2.367992	-2.828022
H	-4.634297	-0.298150	3.699900
H	-4.172248	1.238250	2.937845
H	-3.321161	0.673522	4.394219
H	-1.742203	-1.301037	4.309129
H	-1.436314	-2.160732	2.777511
H	-3.001996	-2.332898	3.595476
H	5.803151	-2.654709	-0.635107
H	2.727175	-3.125877	2.865642
H	1.207462	-2.506097	2.191797
H	1.610355	-2.193733	3.891731
H	3.373369	-0.504470	4.532376
H	4.410700	0.253448	3.300981
H	4.556095	-1.482661	3.647039
C	0.032003	-2.782439	-0.568864
O	0.492565	-3.316487	-1.510982
O	-0.583213	-2.734136	0.477943

$[L^{tBu}Ni(CO_2)]^-$ (singlet state):

	x	y	z
Ni	0.027800	-0.897960	0.000013
H	1.194153	-1.991804	-2.384582
N	-1.541679	0.335788	-0.000007
N	1.434833	0.402756	-0.000002
C	1.941355	-1.635140	-3.104551
C	-1.398972	1.647403	-0.000017
C	-2.752129	-0.403949	0.000000
C	1.202230	1.720976	-0.000016
C	2.710596	-0.246416	0.000005
C	2.654307	-0.372372	-2.586331
H	2.660977	-2.453657	-3.270353
H	1.432005	-1.426618	-4.061306
C	-0.109482	2.248517	-0.000021
C	-2.563304	2.718907	-0.000029
C	-3.320921	-0.834308	-1.228395
C	-3.320935	-0.834269	1.228402
C	2.355669	2.808143	-0.000029

C	3.317894	-0.631355	-1.230737
C	3.317892	-0.631334	1.230753
H	1.882561	0.395210	-2.432457
C	3.625251	0.143763	-3.664680
H	-0.151332	3.324178	-0.000030
C	-4.011849	2.190098	-0.000038
C	-2.428420	3.604944	-1.264570
C	-2.428434	3.604952	1.264509
C	-4.497818	-1.593953	-1.201495
C	-2.654661	-0.536679	-2.570336
C	-4.497832	-1.593915	1.201512
C	-2.654688	-0.536601	2.570340
C	1.828026	4.263754	-0.000042
C	3.244274	2.688815	-1.255676
C	3.244278	2.688836	1.255616
C	4.530758	-1.332304	-1.199878
C	4.530757	-1.332282	1.199907
C	2.654303	-0.372334	2.586344
H	3.065217	0.433813	-4.569823
H	4.344584	-0.633743	-3.971200
H	4.203524	1.018144	-3.330763
H	-4.246588	1.585222	0.882550
H	-4.246569	1.585208	-0.882622
H	-4.692758	3.058548	-0.000052
H	-2.502154	2.995127	-2.178718
H	-1.473985	4.146868	-1.304485
H	-3.241494	4.351058	-1.290787
H	-3.241502	4.351072	1.290708
H	-1.473994	4.146866	1.304433
H	-2.502186	2.995142	2.178660
H	-4.945911	-1.916357	-2.145943
C	-5.103411	-1.959071	0.000010
H	-1.789537	0.110519	-2.367167
C	-3.574592	0.209230	-3.553108
C	-2.113037	-1.831439	-3.204921
H	-4.945935	-1.916290	2.145964
H	-1.789574	0.110608	2.367162
C	-3.574634	0.209310	3.553095
C	-2.113045	-1.831340	3.204952
H	1.228459	4.496220	0.892291
H	1.228453	4.496203	-0.892374
H	2.692740	4.947175	-0.000051
H	2.641914	2.742213	-2.175531
H	3.815101	1.755377	-1.268220
H	3.967979	3.521582	-1.278392
H	3.967978	3.521608	1.278321
H	3.815113	1.755402	1.268168
H	2.641920	2.742240	2.175470
H	4.996553	-1.631087	-2.142434
C	5.149008	-1.674800	0.000018
H	4.996552	-1.631049	2.142469
H	1.882540	0.395228	2.432455
C	1.941379	-1.635106	3.104592
C	3.625239	0.143845	3.664679
H	-6.024258	-2.549281	0.000016
H	-3.946387	1.156591	-3.131649
H	-4.453375	-0.397155	-3.830842
H	-3.033261	0.445738	-4.485015
H	-1.537837	-1.607513	-4.119550
H	-2.935090	-2.512703	-3.483746
H	-1.458221	-2.363226	-2.499566

H	-4.453405	-0.397088	3.830843
H	-3.946449	1.156655	3.131617
H	-3.033308	0.445848	4.484997
H	-1.537853	-1.607389	4.119579
H	-1.458219	-2.363131	2.499610
H	-2.935091	-2.512611	3.483784
H	6.093894	-2.225455	0.000023
H	2.661020	-2.453604	3.270411
H	1.194184	-1.991802	2.384632
H	1.432027	-1.426574	4.061344
H	3.065200	0.433903	4.569817
H	4.203493	1.018229	3.330744
H	4.344588	-0.633641	3.971216
C	0.595844	-2.661877	0.000035
O	1.464837	-3.513280	0.000035
O	-0.688877	-2.672573	0.000050

[L$^{t\text{Bu}}$Ni(N_2)NiL$^{t\text{Bu}}$] (triplet state):

	x	y	z
C	-4.743052	1.133156	0.977219
C	-5.459032	0.359334	0.035228
C	-5.706707	2.031282	1.859053
N	-3.411163	1.057574	1.066763
C	-5.030216	-0.565979	-0.933599
C	-6.680988	1.087666	2.625532
C	-6.518749	2.966908	0.914876
C	-5.066223	2.951584	2.929265
C	-2.629644	1.839417	1.973170
Ni	-2.345412	-0.109711	-0.024877
C	-6.219589	-1.176281	-1.776445
N	-3.728823	-0.851070	-1.068600
C	-2.284982	1.310737	3.242322
C	-2.108741	3.088878	1.552399
N	-0.575933	-0.013444	0.246721
C	-7.194398	-1.898895	-0.800976
C	-6.962819	-0.010950	-2.493105
C	-5.858298	-2.206357	-2.876764
C	-3.184583	-1.777682	-2.012603
C	-1.440968	2.053317	4.075388
C	-2.813245	-0.047931	3.715168
C	-1.269889	3.795994	2.421333
C	-2.441208	3.677654	0.176693
C	-2.376353	-3.365144	0.786336
N	0.567354	0.054606	0.265826
C	-2.751997	-1.316306	-3.281303
C	-2.992850	-3.130853	-1.636355
C	-0.935868	3.288836	3.675174
C	-3.504268	0.040313	5.099163
C	-1.665855	-1.085113	3.769447
C	-3.067504	5.091170	0.284509
C	-1.176219	3.740348	-0.712795
C	-3.478406	-3.619844	-0.269388
Ni	2.346627	0.163643	0.056213
C	-2.107471	-2.212447	-4.140378
C	-2.989869	0.140311	-3.686622
C	-2.350078	-3.993616	-2.530224
C	-3.908451	-5.103511	-0.261065
N	3.422998	-1.163639	0.941095
N	3.717366	1.033885	-0.908407
C	-1.901997	-3.540357	-3.770055

C	-3.206644	0.331252	-5.204185
C	-1.811128	1.009344	-3.189382
C	2.293169	3.395568	1.116500
C	1.836165	-0.707392	-3.272864
C	4.755721	-1.215287	0.830273
C	2.657391	-2.103438	1.701475
C	5.020012	0.738704	-0.824304
C	3.149084	2.011504	-1.784283
C	3.391226	3.734965	0.082273
C	3.026671	0.221805	-3.605426
C	5.461546	-0.298209	0.017963
C	5.735031	-2.236318	1.550445
C	2.089198	-3.231162	1.061216
C	2.389122	-1.848728	3.071479
C	6.198904	1.459965	-1.590303
C	2.735856	1.631678	-3.085976
C	2.911874	3.326549	-1.312270
C	3.798193	5.221792	0.183774
C	3.345753	0.181347	-5.117096
C	6.711319	-1.420662	2.450211
C	6.547537	-3.000549	0.463147
C	5.112521	-3.323247	2.464557
C	1.285360	-4.099390	1.812069
C	2.337969	-3.538004	-0.418888
C	1.573238	-2.736923	3.777264
C	2.987833	-0.617930	3.758016
C	5.819705	2.605154	-2.563417
C	7.157229	2.080829	-0.531686
C	6.966150	0.401964	-2.435844
C	2.053026	2.563053	-3.875481
C	2.230594	4.226962	-2.137666
C	1.025345	-3.860236	3.157661
C	1.006982	-3.583062	-1.206503
C	3.091900	-4.879757	-0.603329
C	2.043693	0.590868	3.559905
C	3.287194	-0.831893	5.258942
C	1.793433	3.849454	-3.406392
H	-6.523159	0.504695	0.063815
H	-7.594520	-1.223535	-0.041460
H	-6.677591	-2.721330	-0.294524
H	-8.032800	-2.315310	-1.372197
H	-7.357078	0.723422	-1.787249
H	-7.799037	-0.419377	-3.073245
H	-6.281600	0.501874	-3.180901
H	-5.210302	-1.782161	-3.644555
H	-6.797356	-2.516224	-3.352601
H	-5.372240	-3.093758	-2.470088
H	-6.118541	0.431230	3.298119
H	-7.271357	0.464458	1.950302
H	-7.368151	1.694390	3.227657
H	-5.842221	3.637484	0.374759
H	-7.202131	3.576554	1.518234
H	-7.109041	2.411351	0.183178
H	-4.514341	2.390304	3.681478
H	-5.884663	3.485246	3.429195
H	-4.392966	3.688484	2.493567
H	-1.179345	1.661387	5.051941
H	-0.285586	3.851466	4.335253
H	-0.875190	4.757580	2.112548
H	-3.165827	3.015334	-0.304850
H	-3.320789	5.464085	-0.715102

H	-2.361706	5.794235	0.740412
H	-3.978372	5.076082	0.890271
H	-1.431257	4.102883	-1.715442
H	-0.711253	2.756047	-0.809286
H	-0.437830	4.421979	-0.279194
H	-3.550412	-0.392542	2.984423
H	-3.907031	-0.941052	5.376663
H	-4.326588	0.762241	5.086050
H	-2.790663	0.343900	5.872883
H	-2.051155	-2.067413	4.068046
H	-0.907246	-0.775333	4.495904
H	-1.180620	-1.185065	2.795636
H	-1.773444	-1.874002	-5.113500
H	-1.403958	-4.222704	-4.449608
H	-2.202875	-5.031675	-2.258891
H	-4.347681	-3.014550	0.006930
H	-4.338581	-5.354371	0.715322
H	-3.052264	-5.766575	-0.427234
H	-4.659019	-5.302379	-1.034189
H	-2.734736	-3.598301	1.795569
H	-2.085656	-2.309720	0.753735
H	-1.490591	-3.969966	0.573372
H	-3.892575	0.481991	-3.169915
H	-3.473519	1.374688	-5.407404
H	-4.012572	-0.313078	-5.572776
H	-2.294432	0.105614	-5.767438
H	-1.997097	2.073408	-3.373167
H	-0.883092	0.719107	-3.690552
H	-1.685326	0.854947	-2.112827
H	6.527687	-0.430137	0.029624
H	7.298604	-0.699361	1.877781
H	7.401120	-2.112235	2.948772
H	6.150243	-0.877877	3.218228
H	7.119013	-2.328663	-0.180387
H	5.873493	-3.589976	-0.166502
H	7.247664	-3.685423	0.956587
H	4.424780	-3.975028	1.926307
H	4.582483	-2.895439	3.314640
H	5.939101	-3.935152	2.847868
H	5.315261	3.428972	-2.057613
H	5.181822	2.261637	-3.378729
H	6.753426	2.987473	-2.995046
H	7.567402	1.327504	0.144694
H	6.622926	2.827730	0.065593
H	7.989325	2.577351	-1.045286
H	7.373730	-0.402994	-1.820379
H	7.795503	0.892329	-2.959657
H	6.297273	-0.039392	-3.182689
H	1.729517	2.284429	-4.871123
H	1.263767	4.559241	-4.031722
H	2.045513	5.235862	-1.789931
H	4.269804	3.126097	0.318939
H	4.223976	5.418222	1.174462
H	2.932125	5.880739	0.057360
H	4.545957	5.479563	-0.574509
H	2.641939	3.577431	2.139493
H	2.026570	2.338490	1.021277
H	1.396204	3.992817	0.932616
H	1.646176	-0.680431	-2.194905
H	2.049777	-1.741245	-3.566619
H	0.932703	-0.371884	-3.790869

H	3.900177	-0.155143	-3.064887
H	3.641907	-0.834635	-5.402703
H	4.163958	0.866321	-5.365566
H	2.469956	0.453719	-5.716137
H	0.862176	-4.975657	1.333622
H	0.401442	-4.543199	3.722960
H	1.370153	-2.557939	4.825762
H	3.931821	-0.385770	3.255737
H	2.480099	1.502470	3.985336
H	1.075855	0.404489	4.033828
H	1.877430	0.747234	2.491831
H	3.810008	0.045833	5.656081
H	3.918277	-1.713824	5.415652
H	2.363600	-0.956963	5.834777
H	2.956304	-2.735251	-0.829869
H	1.200022	-3.731250	-2.274756
H	0.439325	-2.656744	-1.085454
H	0.380749	-4.410467	-0.857179
H	3.267156	-5.068867	-1.669223
H	2.501611	-5.710310	-0.200324
H	4.057930	-4.863470	-0.090848

[L$^{t\mathrm{Bu}}$Ni(CO$_2$)NiL$^{t\mathrm{Bu}}$)] (triplet state):

	x	**y**	**z**
Ni	2.400848	0.000660	0.029321
H	1.731201	0.863100	-2.162194
N	3.914669	0.845069	0.807878
N	3.311495	-1.297308	-0.966902
C	1.742544	0.789052	-3.251349
C	5.180290	0.496279	0.592053
C	3.525697	1.922308	1.668134
C	4.654873	-1.443273	-0.995595
C	2.429276	-2.122214	-1.741942
C	2.611704	-0.421838	-3.661383
H	0.713968	0.673324	-3.602881
H	2.157967	1.716387	-3.664090
C	5.488437	-0.589609	-0.257958
C	6.477846	1.171881	1.196310
C	3.291330	3.207282	1.123522
C	3.265030	1.667328	3.036131
C	5.424141	-2.561472	-1.831850
C	2.052680	-1.713560	-3.048428
C	1.867971	-3.293470	-1.169810
H	3.606105	-0.261976	-3.237386
C	2.746447	-0.479232	-5.200412
H	6.535644	-0.782590	-0.347962
C	6.295282	2.381332	2.148276
C	7.358789	1.678215	0.015306
C	7.260479	0.095716	2.006404
C	2.812756	4.219264	1.963577
C	3.542043	3.513087	-0.356860
C	2.781543	2.707077	3.837343
C	3.490355	0.280074	3.646259
C	6.968556	-2.494545	-1.642149
C	5.191689	-2.419449	-3.359780
C	5.018883	-3.994354	-1.395746
C	1.151039	-2.505303	-3.769516
C	0.977596	-4.056371	-1.934744
C	2.209003	-3.717065	0.265596
H	3.265014	0.419966	-5.552917

H	1.762606	-0.503890	-5.682756
H	3.315416	-1.357844	-5.522056
H	5.737906	2.120896	3.046964
H	5.788949	3.216027	1.665560
H	7.298181	2.712161	2.447643
H	6.818649	2.439118	-0.558170
H	7.643081	0.871716	-0.663756
H	8.272656	2.131366	0.418575
H	8.170868	0.548890	2.417417
H	7.547959	-0.758419	1.389704
H	6.648821	-0.268436	2.838775
H	2.637518	5.208813	1.555584
C	2.557050	3.977348	3.311049
H	3.963771	2.615112	-0.817179
C	4.545006	4.678582	-0.548246
C	2.212009	3.843279	-1.075997
H	2.580188	2.520453	4.886447
H	4.022344	-0.327003	2.908617
C	4.340337	0.332874	4.939692
C	2.131638	-0.402862	3.933335
H	7.259544	-2.654414	-0.598887
H	7.384404	-1.546640	-1.998947
H	7.409285	-3.299609	-2.241039
H	5.505892	-1.429328	-3.706498
H	4.148149	-2.579397	-3.622946
H	5.799344	-3.172964	-3.875954
H	5.634974	-4.714747	-1.947867
H	3.972914	-4.197165	-1.614972
H	5.200149	-4.136776	-0.325127
H	0.868136	-2.211763	-4.772576
C	0.619710	-3.671674	-3.224515
H	0.564770	-4.967392	-1.519177
H	3.213377	-3.347869	0.487435
C	1.243463	-3.041916	1.267873
C	2.198443	-5.249268	0.473854
H	2.184687	4.772917	3.946880
H	5.505148	4.456818	-0.072601
H	4.150979	5.604332	-0.114264
H	4.718458	4.850379	-1.617420
H	2.388212	4.003735	-2.146536
H	1.771001	4.754704	-0.655932
H	1.497334	3.027066	-0.954312
H	3.822761	0.892954	5.726179
H	5.308373	0.809916	4.756729
H	4.517762	-0.684044	5.309775
H	2.285965	-1.416462	4.323280
H	1.542572	-0.460921	3.015560
H	1.567654	0.177184	4.672919
H	-0.066628	-4.279780	-3.803508
H	0.203308	-3.305051	1.053101
H	1.357662	-1.959288	1.187935
H	1.481175	-3.347481	2.293960
H	2.573376	-5.481344	1.477457
H	2.830308	-5.759763	-0.260364
H	1.181517	-5.651126	0.400070
C	0.558645	0.028315	-0.071036
O	-0.642961	-0.275050	-0.389310
O	0.905324	0.951998	0.740925
Ni	-2.470148	-0.142495	-0.023666
N	-3.832936	-0.881337	1.048632
C	-5.138626	-0.518603	1.040750

C	-3.263973	-1.906952	1.876516
C	-5.573300	0.504493	0.196636
C	-6.247156	-1.206015	1.933052
C	-2.712564	-1.559854	3.138044
C	-3.122649	-3.223539	1.365220
C	-4.864210	1.334869	-0.716721
H	-6.622792	0.708118	0.233971
C	-7.658912	-0.597009	1.704676
C	-5.945409	-1.034819	3.445857
C	-6.372538	-2.718490	1.608572
C	-2.757988	-0.113095	3.639459
C	-2.069131	-2.553307	3.884308
C	-2.472485	-4.182081	2.150925
C	-3.604012	-3.570465	-0.047091
N	-3.552888	1.209399	-0.882773
C	-5.827090	2.332991	-1.476411
H	-8.000904	-0.732550	0.673140
H	-7.692485	0.465698	1.966822
H	-8.358919	-1.125915	2.360733
H	-5.878744	0.026272	3.708467
H	-5.020492	-1.534423	3.728624
H	-6.768620	-1.479792	4.017349
H	-7.191986	-3.136518	2.205243
H	-5.458627	-3.256763	1.854246
H	-6.607685	-2.867674	0.549264
C	-1.491763	0.632073	3.156875
H	-3.624715	0.372754	3.184410
C	-2.888526	0.004193	5.175003
H	-1.646142	-2.304018	4.849245
C	-1.955945	-3.855445	3.402864
H	-2.363966	-5.192851	1.777798
H	-4.413551	-2.882624	-0.304470
C	-2.446862	-3.337922	-1.046933
C	-4.136674	-5.015114	-0.180681
C	-2.761203	2.045169	-1.739990
C	-5.195469	3.320429	-2.489834
C	-6.583456	3.202205	-0.427954
C	-6.851930	1.475956	-2.280169
H	-1.400369	0.572777	2.069355
H	-0.593635	0.183815	3.587591
H	-1.528779	1.689927	3.439675
H	-3.013715	1.057710	5.449610
H	-1.986905	-0.363027	5.676891
H	-3.750856	-0.558053	5.548136
H	-1.453774	-4.611137	3.995891
H	-1.604488	-3.997309	-0.823916
H	-2.078246	-2.310825	-0.978477
H	-2.776390	-3.519106	-2.076499
H	-4.550648	-5.159945	-1.185061
H	-4.923197	-5.219709	0.552871
H	-3.333091	-5.746918	-0.045096
C	-2.161995	3.215425	-1.212217
C	-2.495858	1.626347	-3.066592
H	-4.696448	2.807868	-3.310556
H	-4.478801	3.994239	-2.022829
H	-6.013347	3.921530	-2.906413
H	-5.874821	3.805739	0.147462
H	-7.173640	2.602763	0.268334
H	-7.263455	3.879376	-0.957761
H	-7.539511	2.148384	-2.806380
H	-7.438538	0.817799	-1.635345

H	-6.332157	0.862317	-3.023558
C	-1.343366	3.978061	-2.053967
C	-2.382925	3.675423	0.234465
C	-1.667780	2.421541	-3.865475
C	-3.074678	0.326010	-3.634335
H	-0.884851	4.880849	-1.668332
C	-1.100271	3.593504	-3.369988
H	-3.028334	2.942828	0.729028
C	-3.081899	5.058779	0.293106
C	-1.043207	3.749095	1.009421
H	-1.463444	2.118611	-4.885909
H	-3.788730	-0.073397	-2.907291
C	-3.825661	0.547274	-4.970940
C	-1.946253	-0.716734	-3.830433
H	-0.461062	4.197820	-4.003146
H	-4.053246	5.042291	-0.209015
H	-2.458242	5.820718	-0.187185
H	-3.235319	5.353226	1.337974
H	-1.236092	4.001142	2.059311
H	-0.401466	4.529754	0.587737
H	-0.494169	2.805580	0.970544
H	-3.142417	0.914760	-5.743926
H	-4.638095	1.271562	-4.855709
H	-4.251214	-0.401195	-5.319081
H	-2.365629	-1.676965	-4.153526
H	-1.380625	-0.871158	-2.907998
H	-1.245774	-0.370424	-4.598152

[L$^{t\mathrm{Bu}}$Ni(C_2O_4)NiL$^{t\mathrm{Bu}}$] (quintet state):

	x	y	z
Ni	2.643110	0.005739	-0.049585
O	1.137018	-0.149085	1.323590
O	1.127640	0.123686	-1.334760
N	3.953149	1.392972	-0.235000
N	3.824635	-1.501406	-0.239599
C	0.002218	-0.080673	0.775592
C	-0.002451	0.080203	-0.776360
C	3.383633	2.663263	0.107338
C	5.233833	1.180528	-0.557870
C	5.113033	-1.393410	-0.584256
C	3.164198	-2.733603	0.080687
O	-1.127920	-0.123979	1.333973
O	-1.137339	0.148468	-1.324320
C	2.664742	3.404928	-0.869131
C	3.436386	3.117166	1.452957
C	5.710840	-0.128357	-0.773550
C	6.366551	2.273181	-0.715491
C	6.141950	-2.578177	-0.801438
C	2.373014	-3.387946	-0.901005
C	3.207349	-3.232698	1.409724
Ni	-2.643264	-0.005491	0.049025
C	2.103075	4.632136	-0.496517
C	2.490068	2.917691	-2.313505
C	2.849650	4.346162	1.773632
C	4.087680	2.295128	2.571028
H	6.742731	-0.173575	-1.067391
C	7.503808	1.958578	0.300897
C	5.965783	3.751861	-0.483714
C	6.935549	2.188576	-2.163135
C	6.686561	-2.493025	-2.258908

C	5.619214	-4.024829	-0.611914
C	7.325132	-2.401810	0.195981
C	1.733479	-4.585207	-0.557947
C	2.192639	-2.833591	-2.319843
C	2.544705	-4.430161	1.701709
C	3.923871	-2.494119	2.545702
N	-3.953181	-1.392908	0.234168
N	-3.824704	1.501463	0.240475
H	1.568657	5.213332	-1.237978
C	2.205444	5.112318	0.806042
H	2.788945	1.867252	-2.351459
C	1.012800	3.015143	-2.771512
C	3.371236	3.724636	-3.301933
H	2.898781	4.705572	2.795207
H	4.569882	1.423887	2.118257
C	3.002687	1.791885	3.558395
C	5.161902	3.100719	3.344187
H	8.295787	2.709373	0.192927
H	7.940893	0.970860	0.138940
H	7.121898	2.003439	1.325613
H	6.857222	4.364122	-0.669550
H	5.633502	3.932702	0.537646
H	5.178554	4.080081	-1.160639
H	6.154182	2.423317	-2.891904
H	7.337606	1.199835	-2.394966
H	7.742296	2.923319	-2.270795
H	7.421371	-3.292751	-2.409854
H	7.170854	-1.536617	-2.467689
H	5.872494	-2.631657	-2.976259
H	4.795134	-4.259751	-1.283773
H	5.290201	-4.213986	0.408894
H	6.451626	-4.703295	-0.837533
H	6.963937	-2.444664	1.227852
H	7.849584	-1.454418	0.053743
H	8.041387	-3.218378	0.045255
H	1.140167	-5.099080	-1.304294
C	1.830743	-5.117514	0.724379
H	2.560921	-1.804806	-2.328694
C	0.698420	-2.813662	-2.729949
C	2.985203	-3.656057	-3.367950
H	2.586656	-4.825187	2.710345
H	4.430225	-1.622328	2.120873
C	4.981268	-3.381977	3.249146
C	2.887643	-1.997191	3.587752
C	-3.383502	-2.663053	-0.108314
C	-5.233834	-1.180641	0.557223
C	-5.113121	1.393281	0.585015
C	-3.164165	2.733656	-0.079430
H	1.769920	6.069680	1.069789
H	0.341538	2.518857	-2.069842
H	0.902590	2.534891	-3.750392
H	0.700574	4.060747	-2.867466
H	3.122923	4.790856	-3.246903
H	3.190874	3.380526	-4.327321
H	4.434559	3.604866	-3.083153
H	2.503188	2.642682	4.035293
H	3.461830	1.176431	4.341203
H	2.249344	1.193548	3.039733
H	5.941004	3.473237	2.672525
H	5.630850	2.462189	4.102057
H	4.710285	3.956867	3.856822

H	1.334300	-6.050559	0.966382
H	0.319443	-3.830221	-2.880075
H	0.582606	-2.261611	-3.669170
H	0.080010	-2.331889	-1.971158
H	4.060462	-3.612342	-3.182099
H	2.794224	-3.261867	-4.373226
H	2.670017	-4.705576	-3.342380
H	4.504327	-4.244624	3.726885
H	5.493531	-2.804518	4.027780
H	5.728862	-3.751039	2.541114
H	2.135399	-1.363189	3.113041
H	3.391491	-1.424406	4.375719
H	2.381703	-2.851104	4.052418
C	-2.664916	-3.404965	0.868217
C	-3.435741	-3.116637	-1.454072
C	-5.710912	0.128131	0.773633
C	-6.366617	-2.273372	0.714101
C	-6.142050	2.577957	0.802726
C	-2.372670	3.387491	0.902376
C	-3.207352	3.233246	-1.408299
C	-2.103072	-4.632049	0.495480
C	-2.490784	-2.918128	2.312803
C	-2.848879	-4.345546	-1.774839
C	-4.086794	-2.294439	-2.572177
H	-6.742815	0.173145	1.067439
C	-7.503571	-1.958165	-0.302441
C	-5.965823	-3.751943	0.481686
C	-6.936020	-2.189509	2.161613
C	-6.686674	2.492132	2.260140
C	-5.619281	4.024676	0.613890
C	-7.325192	2.402034	-0.194797
C	-1.732789	4.584640	0.559595
C	-2.192448	2.832716	2.321080
C	-2.544342	4.430568	-1.700002
C	-3.924382	2.495315	-2.544390
H	-1.568889	-5.213416	1.236978
C	-2.204984	-5.111928	-0.807226
H	-2.789888	-1.867759	2.350996
C	-1.013643	-3.015423	2.771243
C	-3.372098	-3.725568	3.300705
H	-2.897667	-4.704706	-2.796520
H	-4.568810	-1.423088	-2.119403
C	-3.001739	-1.791431	-3.559604
C	-5.161198	-3.099810	-3.345339
H	-8.295600	-2.709010	-0.195164
H	-7.940665	-0.970531	-0.139990
H	-7.121365	-2.002400	-1.327074
H	-6.857333	-4.364276	0.666947
H	-5.633238	-3.932281	-0.539657
H	-5.178803	-4.080502	1.158686
H	-6.154888	-2.424674	2.890498
H	-7.338132	-1.200890	2.393878
H	-7.742831	-2.924275	2.268634
H	-7.421547	3.291737	2.411432
H	-7.170902	1.535595	2.468485
H	-5.872627	2.630501	2.977570
H	-4.795190	4.259235	1.285854
H	-5.290276	4.214311	-0.406828
H	-6.451668	4.703063	0.839842
H	-6.963972	2.445169	-1.226652
H	-7.849731	1.454642	-0.052858

H	-8.041393	3.218613	-0.043854
H	-1.139212	5.098092	1.306020
C	-1.830005	5.117367	-0.722560
H	-2.560909	1.803990	2.329614
C	-0.698278	2.812406	2.731326
C	-2.984983	3.655026	3.369340
H	-2.586302	4.825928	-2.708507
H	-4.431073	1.623635	-2.119732
C	-4.981497	3.383844	-3.247415
C	-2.888580	1.998189	-3.586783
H	-1.769353	-6.069219	-1.071053
H	-0.342304	-2.518477	2.070118
H	-0.903915	-2.535743	3.750465
H	-0.701119	-4.060983	2.866663
H	-3.123503	-4.791710	3.245464
H	-3.192165	-3.381698	4.326248
H	-4.435374	-3.606000	3.081595
H	-2.502562	-2.642332	-4.036650
H	-3.460811	-1.175798	-4.342314
H	-2.248192	-1.193357	-3.040953
H	-5.940446	-3.472111	-2.673735
H	-5.629932	-2.461219	-4.103293
H	-4.709727	-3.956097	-3.857876
H	-1.333250	6.050302	-0.964343
H	-0.319093	3.828854	2.881705
H	-0.582686	2.260161	3.670466
H	-0.079902	2.330607	1.972524
H	-4.060240	3.611452	3.183434
H	-2.794099	3.260574	4.374533
H	-2.669691	4.704518	3.344038
H	-4.504219	4.246331	-3.725109
H	-5.494221	2.806792	-4.026049
H	-5.728756	3.753171	-2.539166
H	-2.136511	1.363729	-3.112415
H	-3.392858	1.425849	-4.374801
H	-2.382374	2.852013	-4.051322

[$L^{tBu}Ni(N_2)$] (doublet state):

	x	**y**	**z**
C	1.186975	0.000064	1.589549
C	-0.113413	0.000100	2.152148
C	2.314206	0.000101	2.702074
N	1.373865	0.000001	0.265645
C	-1.397041	0.000076	1.572130
C	2.138557	-1.272998	3.582166
C	2.138580	1.273268	3.582070
C	3.791035	0.000070	2.231856
C	2.654729	-0.000015	-0.371454
Ni	-0.105874	-0.000071	-0.955221
C	-2.565227	0.000128	2.631200
N	-1.538091	0.000010	0.240896
C	3.247407	-1.228485	-0.761489
C	3.247397	1.228435	-0.761566
N	0.648223	-0.000068	-2.569895
C	-2.428938	-1.273329	3.515656
C	-2.428935	1.273667	3.515536
C	-4.013414	0.000102	2.079994
C	-2.774550	-0.000028	-0.479644
C	4.446327	-1.202923	-1.482887
C	2.603007	-2.580557	-0.434654

C	4.446318	1.202837	-1.482962
C	2.602985	2.580523	-0.434820
C	-1.664638	-2.927435	-1.599039
N	1.086716	-0.000030	-3.600755
C	-3.351528	1.229334	-0.887780
C	-3.351512	-1.229433	-0.887670
C	5.052317	-0.000052	-1.836529
C	3.550157	-3.491206	0.387079
C	2.180683	-3.311671	-1.734815
C	3.550119	3.491223	0.386876
C	2.180680	3.311563	-1.735029
C	-2.692324	-2.554479	-0.501360
C	-4.496262	1.205542	-1.691115
C	-2.692357	2.554423	-0.501588
C	-4.496247	-1.205728	-1.691006
C	-3.697646	-3.705224	-0.276196
C	-5.069430	-0.000115	-2.090400
C	-3.697693	3.705181	-0.276551
C	-1.664657	2.927283	-1.599285
H	-0.122593	0.000150	3.226748
H	-1.468673	-1.313953	4.034734
H	-2.525859	-2.172334	2.896954
H	-3.229725	-1.279621	4.264835
H	-1.468670	1.314338	4.034611
H	-3.229722	1.280032	4.264715
H	-2.525854	2.172615	2.896751
H	-4.226797	0.884281	1.477868
H	-4.690924	0.000150	2.943154
H	-4.226801	-0.884140	1.477962
H	2.268934	-2.173701	2.972976
H	1.156098	-1.317905	4.056986
H	2.903273	-1.272653	4.368228
H	2.268971	2.173924	2.972812
H	2.903299	1.272969	4.368131
H	1.156124	1.318228	4.056891
H	4.038566	-0.882018	1.642926
H	4.418235	0.000098	3.132446
H	4.038582	0.882107	1.642858
H	4.908200	-2.139359	-1.775807
H	5.981433	-0.000066	-2.394851
H	4.908184	2.139258	-1.775940
H	1.704527	2.390935	0.159265
H	3.047954	4.436632	0.624272
H	4.457280	3.720931	-0.182663
H	3.844688	3.010077	1.324211
H	1.694001	4.263874	-1.492497
H	1.482347	2.702791	-2.315455
H	3.056815	3.520015	-2.358654
H	1.704559	-2.390939	0.159436
H	3.048000	-4.436603	0.624537
H	3.844738	-3.010004	1.324382
H	4.457311	-3.720944	-0.182460
H	1.694011	-4.263971	-1.492224
H	3.056808	-3.520152	-2.358445
H	1.482337	-2.702932	-2.315261
H	-4.946111	2.138816	-2.007013
H	-5.957248	-0.000148	-2.712456
H	-4.946084	-2.139037	-2.006819
H	-2.141716	-2.394886	0.431105
H	-3.165608	-4.591312	0.088482
H	-4.203414	-3.981080	-1.207828

H	-4.456629	-3.425701	0.462878
H	-1.115424	-3.838646	-1.335914
H	-0.948075	-2.104198	-1.701843
H	-2.171378	-3.075979	-2.558905
H	-2.141763	2.394925	0.430901
H	-3.165670	4.591309	0.088049
H	-4.456685	3.425722	0.462539
H	-4.203449	3.980940	-1.208219
H	-1.115455	3.838523	-1.336238
H	-2.171384	3.075733	-2.559173
H	-0.948088	2.104042	-1.702000

[L$^{t\text{Bu}}$Ni] (doublet state):

	x	y	z
Ni	0.029882	0.292387	-0.919392
H	1.144818	2.395290	-0.717106
N	-1.472335	0.195045	0.145144
N	1.506009	-0.118400	0.104619
C	1.903689	3.114641	-0.390382
C	-1.273445	0.033257	1.464382
C	-2.720318	0.130967	-0.540608
C	1.298288	-0.405441	1.398614
C	2.771644	0.012893	-0.540329
C	2.961082	2.357531	0.452584
H	2.375692	3.566936	-1.269819
H	1.414028	3.897886	0.200561
C	0.011658	-0.260721	1.981004
C	-2.371305	0.239113	2.575584
C	-3.242770	1.305545	-1.144895
C	-3.361059	-1.117082	-0.760551
C	2.381223	-0.963126	2.400015
C	3.514420	1.215074	-0.401528
C	3.213633	-0.992876	-1.435272
H	2.445669	1.920368	1.312379
C	4.037203	3.329611	0.980573
H	0.011872	-0.419780	3.045890
C	-3.796966	0.567091	2.067237
C	-1.920876	1.459166	3.434878
C	-2.483266	-1.016124	3.483799
C	-4.396889	1.218079	-1.927907
C	-2.514376	2.639044	-0.971317
C	-4.516336	-1.155648	-1.550512
C	-2.796678	-2.426647	-0.202160
C	2.537575	-0.001039	3.611056
C	3.798752	-1.195560	1.819693
C	1.882370	-2.351596	2.901159
C	4.706363	1.361201	-1.117851
C	4.409690	-0.803268	-2.135820
C	2.353063	-2.235010	-1.667762
H	3.572270	4.057293	1.655387
H	4.505259	3.887757	0.162000
H	4.819328	2.794944	1.531245
H	-4.238372	-0.258460	1.508108
H	-3.807830	1.455732	1.432876
H	-4.424614	0.765296	2.945204
H	-1.847081	2.353125	2.805308
H	-0.949176	1.286463	3.903289
H	-2.663960	1.645109	4.220109
H	-3.240880	-0.834456	4.255884
H	-1.539318	-1.249776	3.982543

H	-2.789488	-1.887131	2.897027
H	-4.803434	2.112992	-2.382491
C	-5.038716	-0.002689	-2.129110
H	-2.030522	2.626478	0.012311
C	-3.442636	3.871415	-1.042927
C	-1.398575	2.738581	-2.041428
H	-5.008704	-2.106640	-1.720180
H	-1.989785	-2.181920	0.492810
C	-3.867412	-3.248554	0.557377
C	-2.198081	-3.277473	-1.351093
H	1.598145	0.136249	4.152267
H	2.890336	0.979320	3.274618
H	3.277711	-0.414932	4.306539
H	4.277531	-0.267020	1.507309
H	3.783070	-1.878008	0.967610
H	4.408214	-1.649624	2.611270
H	2.617126	-2.769708	3.600073
H	1.777059	-3.038893	2.054149
H	0.917631	-2.279905	3.407999
H	5.285564	2.269727	-1.010547
C	5.160319	0.358445	-1.973137
H	4.760894	-1.572904	-2.811814
H	1.832607	-2.460938	-0.729953
C	1.278912	-1.886874	-2.729507
C	3.154909	-3.483385	-2.094655
H	-5.934811	-0.054028	-2.736913
H	-4.272020	3.778204	-0.333544
H	-3.856758	4.002067	-2.048703
H	-2.873034	4.774766	-0.797044
H	-0.872706	3.698520	-1.989905
H	-1.806769	2.594307	-3.046312
H	-0.653679	1.950494	-1.828770
H	-4.661306	-3.579242	-0.121066
H	-4.323560	-2.657227	1.357530
H	-3.408565	-4.140589	1.000040
H	-1.774953	-4.208756	-0.955378
H	-1.405450	-2.724430	-1.863090
H	-2.974380	-3.529318	-2.082286
H	6.088804	0.487284	-2.517695
H	1.746481	-1.531861	-3.653296
H	0.640471	-1.088110	-2.310183
H	0.635766	-2.745889	-2.949430
H	2.487078	-4.351133	-2.138220
H	3.957753	-3.697373	-1.380650
H	3.597023	-3.353163	-3.088545

[L$^{t\text{Bu}}$Ni(CO)] (doublet state):

	x	**y**	**z**
Ni	0.106269	0.000009	-0.966838
H	0.953494	2.170482	-1.731448
N	-1.364900	0.000008	0.268588
N	1.536482	0.000013	0.245023
C	1.685522	2.974982	-1.596543
C	-1.177688	0.000021	1.593151
C	-2.651834	-0.000002	-0.359819
C	1.402821	0.000025	1.575953
C	2.765759	-0.000008	-0.487444
C	2.692708	2.556702	-0.496347
H	2.207001	3.137522	-2.546243
H	1.153106	3.891501	-1.317110

C	0.121125	0.000030	2.158135
C	-2.304813	0.000031	2.707575
C	-3.248501	1.228895	-0.741899
C	-3.248491	-1.228911	-0.741878
C	2.575018	0.000041	2.629228
C	3.337204	1.229816	-0.901501
C	3.337190	-1.229855	-0.901454
H	2.128317	2.386050	0.425699
C	3.716831	3.682828	-0.231356
H	0.130358	0.000042	3.232604
C	-3.783612	0.000025	2.242851
C	-2.126886	1.273088	3.587554
C	-2.126881	-1.273009	3.587578
C	-4.462735	1.203018	-1.437083
C	-2.589884	2.580153	-0.441245
C	-4.462726	-1.203055	-1.437060
C	-2.589865	-2.580159	-0.441200
C	2.442362	1.273489	3.514112
C	4.019516	0.000039	2.069009
C	2.442371	-1.273380	3.514149
C	4.467184	1.205732	-1.725380
C	4.467171	-1.205814	-1.725333
C	2.692678	-2.556718	-0.496253
H	3.196562	4.572240	0.142202
H	4.244031	3.966335	-1.148613
H	4.457437	3.373122	0.514291
H	-4.033761	-0.882133	1.655187
H	-4.033764	0.882173	1.655174
H	-4.406636	0.000031	3.146312
H	-2.259033	2.173950	2.979223
H	-1.143690	1.318377	4.060742
H	-2.890052	1.271983	4.375038
H	-2.890047	-1.271892	4.375063
H	-1.143685	-1.318286	4.060765
H	-2.259027	-2.173883	2.979264
H	-4.928873	2.139283	-1.723529
C	-5.077396	-0.000024	-1.774730
H	-1.672735	2.390021	0.123282
C	-3.506645	3.497543	0.406627
C	-2.207676	3.303564	-1.758216
H	-4.928858	-2.139329	-1.723488
H	-1.672708	-2.390010	0.123308
C	-3.506611	-3.497530	0.406711
C	-2.207675	-3.303607	-1.758156
H	1.484580	1.313470	4.037937
H	2.536046	2.172691	2.895264
H	3.246618	1.279806	4.259492
H	4.228853	0.884274	1.465499
H	4.228862	-0.884214	1.465529
H	4.702704	0.000057	2.927629
H	3.246628	-1.279671	4.259529
H	2.536062	-2.172600	2.895327
H	1.484590	-1.313354	4.037975
H	4.911771	2.139119	-2.048650
C	5.031752	-0.000052	-2.136544
H	4.911749	-2.139218	-2.048566
H	2.128285	-2.386027	0.425783
C	1.685492	-2.975027	-1.596439
C	3.716786	-3.682846	-0.231218
H	-6.018729	-0.000032	-2.312164
H	-3.768441	3.023814	1.357373

H	-4.433114	3.723407	-0.132599
H	-2.996139	4.444381	0.619153
H	-1.701077	4.250346	-1.535890
H	-3.103772	3.521265	-2.349439
H	-1.539579	2.684842	-2.363532
H	-4.433088	-3.723408	-0.132495
H	-3.768391	-3.023778	1.357449
H	-2.996101	-4.444362	0.619251
H	-1.701065	-4.250378	-1.535809
H	-1.539595	-2.684900	-2.363504
H	-3.103780	-3.521334	-2.349356
H	5.907153	-0.000069	-2.775932
H	2.206974	-3.137610	-2.546130
H	0.953475	-2.170523	-1.731380
H	1.153063	-3.891528	-1.316974
H	3.196505	-4.572240	0.142368
H	4.457392	-3.373124	0.514421
H	4.243988	-3.966392	-1.148462
C	-0.650380	-0.000030	-2.560000
O	-1.132701	-0.000081	-3.607980

$[L^{tBu}NiO]^-$ (triplet state):

	x	y	z
Ni	0.020256	0.208683	-1.038828
H	1.109569	2.494846	-1.446929
N	-1.434570	-0.022512	0.237543
N	1.431139	-0.111577	0.262570
C	1.741936	3.240436	-0.948286
C	-1.306154	-0.234439	1.544375
C	-2.683115	0.054521	-0.441662
C	1.259906	-0.411581	1.559599
C	2.693692	0.088437	-0.368770
C	2.529245	2.578069	0.214608
H	2.445031	3.648186	-1.684631
H	1.112192	4.056263	-0.568880
C	-0.029081	-0.438796	2.127509
C	-2.472485	-0.291127	2.617293
C	-3.241342	1.310869	-0.779276
C	-3.310948	-1.137535	-0.888927
C	2.446667	-0.770898	2.543795
C	3.291405	1.380895	-0.359457
C	3.293934	-0.943214	-1.141946
H	1.804372	2.199020	0.939910
C	3.430250	3.618582	0.917861
H	-0.059305	-0.646762	3.178102
C	-3.917432	-0.043287	2.114658
C	-2.197247	0.805156	3.688707
C	-2.473790	-1.693809	3.290067
C	-4.453433	1.350199	-1.476894
C	-2.506462	2.613843	-0.462934
C	-4.520503	-1.053254	-1.583872
C	-2.596992	-2.478990	-0.719091
C	1.963642	-1.201629	3.956757
C	3.389287	0.441922	2.760583
C	3.261303	-1.966889	1.986549
C	4.516766	1.575721	-1.004456
C	4.520154	-0.701875	-1.771752
C	2.556422	-2.257965	-1.408334
H	2.805099	4.405559	1.357626
H	4.110083	4.097007	0.203364

H	4.026761	3.160419	1.714431
H	-4.242046	-0.800249	1.400619
H	-4.021384	0.932978	1.640034
H	-4.580488	-0.078086	2.990529
H	-2.201307	1.793932	3.216299
H	-1.233392	0.664267	4.182468
H	-2.989470	0.777898	4.448636
H	-3.264273	-1.732133	4.051333
H	-1.517739	-1.919577	3.768185
H	-2.676243	-2.466369	2.540074
H	-4.883342	2.312829	-1.732855
C	-5.106382	0.181753	-1.861552
H	-1.650953	2.363851	0.170684
C	-3.397205	3.627062	0.295271
C	-1.956728	3.216481	-1.781816
H	-5.004924	-1.961736	-1.923849
H	-1.923279	-2.395418	0.138295
C	-3.548650	-3.669994	-0.472414
C	-1.727905	-2.708331	-1.983323
H	1.297762	-2.069452	3.906773
H	1.455521	-0.384345	4.480029
H	2.847450	-1.479452	4.544755
H	2.826257	1.288749	3.169358
H	3.857800	0.747824	1.826296
H	4.173847	0.165283	3.477914
H	4.048253	-2.234230	2.704427
H	3.725316	-1.714910	1.034687
H	2.607881	-2.835212	1.844236
H	4.972344	2.559419	-0.990725
C	5.148805	0.537526	-1.685955
H	4.978073	-1.492899	-2.355367
H	1.760738	-2.349398	-0.663389
C	1.896082	-2.168371	-2.811316
C	3.463971	-3.507496	-1.319611
H	-6.048027	0.231630	-2.398326
H	-3.771569	3.198996	1.232981
H	-4.257249	3.925715	-0.315547
H	-2.819147	4.529613	0.529835
H	-1.397263	4.138119	-1.572344
H	-2.784369	3.455209	-2.461517
H	-1.289087	2.483686	-2.258003
H	-4.193730	-3.848584	-1.340345
H	-4.184996	-3.492754	0.403121
H	-2.962406	-4.581047	-0.300111
H	-1.110771	-3.609976	-1.876457
H	-1.077397	-1.839029	-2.137120
H	-2.373148	-2.817162	-2.863029
H	6.102314	0.704099	-2.176232
H	2.671801	-2.058420	-3.578772
H	1.228529	-1.297331	-2.852495
H	1.318958	-3.079137	-3.018656
H	2.859166	-4.411039	-1.466320
H	3.961725	-3.574707	-0.346364
H	4.230831	-3.490662	-2.102715
O	-0.013648	0.721029	-2.644197

$[L^{tBu}Ni(C(O)OC(O)O)NiL^{tBu}]^{2-}$ (open-shell singlet state):

	x	y	z
N	4.158064	1.510472	0.463449
C	5.514498	1.533442	0.524995
C	3.325546	2.533231	0.983902
C	6.267622	0.368984	0.269875
C	6.356914	2.837658	0.850368
C	2.991799	2.546615	2.370089
C	2.679088	3.451070	0.108144
C	5.899666	-0.948436	-0.108697
H	7.325522	0.490730	0.400138
C	7.883935	2.649821	0.618506
C	6.199257	3.276698	2.331649
C	5.938823	4.021296	-0.061480
C	3.550855	1.468025	3.304983
C	2.077193	3.489168	2.848485
C	1.768295	4.374169	0.631680
C	2.936452	3.390932	-1.401663
N	4.616565	-1.261513	-0.376377
C	7.145110	-1.933368	-0.120605
H	8.091429	2.319578	-0.404524
H	8.317491	1.931584	1.322971
H	8.375255	3.618619	0.781328
H	6.516956	2.468055	2.999351
H	5.162826	3.530660	2.553288
H	6.830334	4.157336	2.521502
H	6.573220	4.891256	0.161011
H	4.898785	4.295878	0.107441
H	6.070451	3.753363	-1.115599
C	2.581919	0.259106	3.331941
H	4.497441	1.122191	2.881601
C	3.812375	1.972659	4.743678
H	1.815259	3.490524	3.900848
C	1.470977	4.408255	1.992797
H	1.267949	5.064176	-0.037745
H	3.933480	2.964781	-1.541901
C	1.930956	2.430831	-2.083088
C	2.897122	4.780309	-2.081504
C	4.219128	-2.510418	-0.917084
C	6.901653	-3.398378	-0.566551
C	7.714293	-2.008717	1.327415
C	8.245212	-1.381118	-1.075802
H	2.429119	-0.108388	2.315421
H	1.605171	0.560176	3.725578
H	2.992268	-0.545482	3.957795
H	4.296705	1.178845	5.326780
H	2.872016	2.226403	5.247109
H	4.461010	2.856202	4.748168
H	0.755996	5.127869	2.380006
H	0.899484	2.733716	-1.877878
H	2.085832	1.423886	-1.692782
H	2.096820	2.416232	-3.169398
H	3.207791	4.683473	-3.129628
H	3.565587	5.490933	-1.580750
H	1.880370	5.190576	-2.073804
C	3.679264	-3.519483	-0.075349
C	4.236561	-2.717879	-2.322574
H	6.548697	-3.459805	-1.596450
H	6.170296	-3.901786	0.064030
H	7.860258	-3.932779	-0.488472
H	6.956351	-2.427943	1.998508

H	7.989200	-1.018473	1.698644
H	8.601230	-2.659006	1.349063
H	9.110534	-2.059468	-1.068170
H	8.584108	-0.384636	-0.784365
H	7.853757	-1.326455	-2.097003
C	3.247188	-4.723997	-0.638822
C	3.534138	-3.301137	1.433736
C	3.795433	-3.937593	-2.843968
C	4.652933	-1.593523	-3.274624
H	2.833662	-5.491173	0.008522
C	3.317620	-4.949089	-2.012377
H	3.965909	-2.323296	1.663685
C	4.290415	-4.378554	2.252634
C	2.040522	-3.277530	1.843776
H	3.805609	-4.089044	-3.919212
H	5.048592	-0.778140	-2.663547
C	5.748612	-2.036613	-4.274790
C	3.405728	-1.067556	-4.031387
H	2.973297	-5.888828	-2.432770
H	5.357204	-4.387454	2.003377
H	3.879348	-5.375729	2.052801
H	4.184311	-4.175062	3.326121
H	1.948017	-3.115418	2.925407
H	1.557121	-4.229019	1.592232
H	1.503025	-2.474892	1.334907
H	5.385941	-2.850612	-4.914347
H	6.643981	-2.383959	-3.747037
H	6.029351	-1.195322	-4.922221
H	3.670795	-0.196102	-4.645997
H	2.633211	-0.790373	-3.308850
H	3.005177	-1.850335	-4.688401
Ni	3.188245	-0.026431	-0.109492
Ni	-3.193517	-0.024931	-0.022233
C	-1.532082	-0.826546	0.474077
O	-0.490665	-0.664433	-0.753904
O	-1.040724	-1.325062	1.447549
C	0.807103	-0.428273	-0.482001
O	1.164413	0.346260	0.462886
O	1.696646	-0.956869	-1.238100
H	-2.408310	-0.060818	-2.217766
N	-4.614905	-1.272747	0.382781
N	-4.255069	1.477334	-0.491951
C	-2.505277	0.295049	-3.248379
C	-5.904515	-0.974961	0.211387
C	-4.163295	-2.530337	0.872271
C	-5.599539	1.489767	-0.500985
C	-3.428007	2.531052	-0.980183
C	-3.531838	1.453534	-3.302792
H	-1.517503	0.635136	-3.575099
H	-2.828909	-0.541718	-3.881356
C	-6.324656	0.328755	-0.169894
C	-7.143479	-1.964346	0.350623
C	-3.672666	-3.514580	-0.025522
C	-4.073853	-2.753265	2.271791
C	-6.466196	2.764489	-0.869558
C	-3.062046	2.562476	-2.356285
C	-2.837042	3.460314	-0.078779
H	-4.483699	1.071208	-2.924086
C	-3.740462	1.926214	-4.759381
H	-7.388891	0.432519	-0.235728
C	-6.860133	-3.424122	0.789966

C	-7.839202	-2.058879	-1.040031
C	-8.151907	-1.392858	1.390900
C	-3.203372	-4.728435	0.486863
C	-3.626329	-3.274315	-1.538680
C	-3.593940	-3.980957	2.738216
C	-4.426857	-1.653255	3.278535
C	-7.991072	2.544918	-0.660320
C	-6.288935	3.157829	-2.360777
C	-6.087755	3.977805	0.020683
C	-2.180320	3.549712	-2.807460
C	-1.958757	4.428303	-0.576924
C	-3.084339	3.340636	1.427893
H	-4.159222	1.103845	-5.352704
H	-2.788383	2.214445	-5.219326
H	-4.426776	2.779747	-4.809653
H	-6.420135	-3.474794	1.785330
H	-6.187198	-3.936132	0.103597
H	-7.822168	-3.956992	0.801230
H	-7.144591	-2.483610	-1.772512
H	-8.159684	-1.078479	-1.399595
H	-8.716907	-2.716330	-0.967906
H	-9.010169	-2.073928	1.474174
H	-8.521055	-0.403948	1.110724
H	-7.672490	-1.316418	2.371875
H	-2.832358	-5.481888	-0.200163
C	-3.178710	-4.976881	1.857306
H	-3.977257	-2.254475	-1.718012
C	-4.548862	-4.258972	-2.302439
C	-2.177589	-3.382566	-2.078900
H	-3.522458	-4.148801	3.808093
H	-4.836342	-0.810053	2.716154
C	-5.480141	-2.114977	4.316295
C	-3.142935	-1.172179	4.002695
H	-8.216242	2.266128	0.374398
H	-8.387616	1.779034	-1.335549
H	-8.502933	3.489978	-0.883940
H	-6.575204	2.321455	-3.008303
H	-5.256260	3.432276	-2.573643
H	-6.938124	4.014992	-2.588309
H	-6.736059	4.827183	-0.235401
H	-5.050576	4.271466	-0.133191
H	-6.235219	3.733279	1.078408
H	-1.892182	3.569212	-3.851959
C	-1.639044	4.488422	-1.931493
H	-1.495558	5.126737	0.108710
H	-4.080271	2.909655	1.565394
C	-2.060574	2.343981	2.025071
C	-3.028390	4.693605	2.172877
H	-2.803095	-5.921887	2.235859
H	-5.589854	-4.162332	-1.976362
H	-4.227298	-5.293880	-2.132804
H	-4.501504	-4.057891	-3.380441
H	-2.172870	-3.205542	-3.162644
H	-1.767843	-4.382552	-1.893683
H	-1.526329	-2.640903	-1.608734
H	-5.094753	-2.952533	4.909995
H	-6.406155	-2.435876	3.827409
H	-5.715241	-1.291719	5.003437
H	-3.366906	-0.303287	4.636023
H	-2.377464	-0.909938	3.268635
H	-2.745806	-1.973849	4.638193

H	-0.945215	5.238763	-2.295961
H	-1.032143	2.673526	1.849526
H	-2.201437	1.376191	1.533532
H	-2.227211	2.216354	3.102751
H	-3.325075	4.544692	3.218462
H	-3.700312	5.432434	1.718766
H	-2.009152	5.096141	2.173185

$[L^{tBu}Ni(CO)(OC(O)O)NiL^{tBu}]^{2-}$ (open-shell singlet state):

	x	y	z
N	-4.060303	1.287834	-0.212313
C	-5.383282	0.947541	-0.197971
C	-3.593125	2.555248	-0.639139
C	-5.784102	-0.401673	-0.119365
C	-6.562686	2.007431	-0.220602
C	-3.470948	2.843750	-2.032389
C	-3.108504	3.508314	0.303640
C	-5.068595	-1.613085	0.049914
H	-6.843571	-0.548944	-0.211974
C	-7.949681	1.380960	0.106028
C	-6.716262	2.689206	-1.607711
C	-6.342545	3.108866	0.848384
C	-3.831030	1.774979	-3.070627
C	-2.939316	4.070079	-2.440319
C	-2.573856	4.718473	-0.153031
C	-3.139239	3.210861	1.807259
N	-3.728758	-1.610110	0.250243
C	-6.000226	-2.888367	-0.099733
H	-7.924641	0.843660	1.059379
H	-8.285439	0.697570	-0.681785
H	-8.683944	2.195001	0.177785
H	-6.903967	1.932910	-2.378275
H	-5.814651	3.242638	-1.869703
H	-7.568073	3.385046	-1.583478
H	-7.200250	3.796993	0.844281
H	-5.438281	3.676951	0.639187
H	-6.257739	2.659631	1.843967
C	-2.573357	0.925777	-3.387123
H	-4.574336	1.113131	-2.618795
C	-4.418489	2.354411	-4.379316
H	-2.843613	4.282598	-3.499569
C	-2.500640	5.014365	-1.512146
H	-2.198619	5.436480	0.567934
H	-3.895863	2.437780	1.966220
C	-1.781103	2.637554	2.282374
C	-3.513313	4.450366	2.658007
C	-3.021478	-2.742531	0.721207
C	-5.352263	-4.276909	0.133369
C	-6.555436	-2.903762	-1.555325
C	-7.191530	-2.808644	0.900829
H	-2.169413	0.503937	-2.465391
H	-1.796401	1.554560	-3.837387
H	-2.826346	0.114088	-4.083373
H	-4.738051	1.531275	-5.031360
H	-3.664528	2.934791	-4.924466
H	-5.281616	2.999967	-4.181834
H	-2.084853	5.959866	-1.846938
H	-0.955888	3.301567	2.006372
H	-1.613910	1.659686	1.829308
H	-1.787815	2.510555	3.374279

H	-3.637391	4.149237	3.706107
H	-4.446063	4.909890	2.311813
H	-2.717786	5.204041	2.621764
C	-2.249827	-3.533035	-0.173124
C	-2.982520	-3.033773	2.111774
H	-4.968725	-4.384131	1.149170
H	-4.528765	-4.462327	-0.554662
H	-6.127514	-5.039327	-0.035445
H	-5.723024	-2.987974	-2.263038
H	-7.102079	-1.983986	-1.778554
H	-7.226346	-3.764446	-1.696223
H	-7.838325	-3.688371	0.770628
H	-7.796810	-1.911241	0.755092
H	-6.811281	-2.804508	1.927581
C	-1.502018	-4.603426	0.325256
C	-2.228846	-3.219623	-1.671914
C	-2.236454	-4.125729	2.566426
C	-3.677735	-2.118241	3.122571
H	-0.895451	-5.190014	-0.355967
C	-1.505799	-4.919323	1.683529
H	-3.065502	-2.543090	-1.871880
C	-2.403541	-4.488217	-2.544843
C	-0.918917	-2.486805	-2.057136
H	-2.207423	-4.342192	3.630200
H	-4.284975	-1.407589	2.556624
C	-4.605046	-2.896439	4.087402
C	-2.611114	-1.318685	3.915402
H	-0.924040	-5.758788	2.052323
H	-3.314792	-5.033702	-2.273273
H	-1.546852	-5.162395	-2.430534
H	-2.467686	-4.202408	-3.602612
H	-0.883250	-2.320904	-3.142873
H	-0.046342	-3.079118	-1.760645
H	-0.868363	-1.514069	-1.562869
H	-4.032522	-3.618031	4.683040
H	-5.377407	-3.441075	3.532466
H	-5.097637	-2.200086	4.778948
H	-3.095590	-0.591841	4.582261
H	-1.952250	-0.796127	3.216016
H	-2.003593	-2.001003	4.524105
Ni	-2.691459	-0.014443	0.093191
Ni	2.560458	0.150608	-0.627149
O	1.027062	0.302438	0.545546
C	-0.250432	0.183682	0.345465
O	-0.858258	0.721743	-0.662246
O	-0.992461	-0.474004	1.184683
O	2.345728	0.685184	-3.461557
C	2.263604	0.257017	-2.377039
H	1.630641	0.510858	2.605798
N	3.970802	-1.275259	-0.428714
N	3.692260	1.661498	0.137170
C	2.165573	0.870530	3.489624
C	5.246306	-0.984307	-0.217580
C	3.442253	-2.596034	-0.512807
C	5.024426	1.585577	0.060191
C	3.005484	2.767449	0.727399
C	3.389122	1.726470	3.066476
H	1.478623	1.482261	4.087859
H	2.492741	0.016277	4.097688
C	5.699772	0.360398	-0.150069
C	6.446971	-2.011418	-0.021406

C	2.872377	-3.211243	0.636812
C	3.377537	-3.271717	-1.764862
C	5.997737	2.840374	0.186781
C	2.894550	2.851565	2.148357
C	2.308541	3.723113	-0.068456
H	4.072544	1.093740	2.494442
C	4.120006	2.228144	4.337897
H	6.767180	0.443352	-0.152729
C	6.103137	-3.522915	-0.025689
C	7.121951	-1.721719	1.351538
C	7.493863	-1.793177	-1.153531
C	2.375794	-4.516047	0.534732
C	2.777685	-2.497269	1.990310
C	2.866667	-4.573517	-1.814653
C	3.818838	-2.616317	-3.078170
C	7.452505	2.542442	-0.280679
C	6.101710	3.335940	1.650000
C	5.501056	3.999090	-0.708699
C	2.205112	3.923600	2.725655
C	1.622683	4.770696	0.558734
C	2.217288	3.618055	-1.594487
H	4.487809	1.365309	4.908016
H	3.431415	2.782668	4.986149
H	4.968757	2.874803	4.097483
H	5.681099	-3.847078	-0.975531
H	5.393305	-3.782318	0.758834
H	7.037696	-4.074907	0.150590
H	6.402816	-1.880658	2.160930
H	7.486069	-0.694353	1.414288
H	7.966598	-2.410021	1.494338
H	8.320880	-2.504008	-1.019854
H	7.903412	-0.780697	-1.145748
H	7.036209	-1.971795	-2.130813
H	1.948709	-4.983082	1.414294
C	2.389734	-5.209825	-0.671737
H	3.079897	-1.457609	1.843136
C	3.721238	-3.146970	3.037080
C	1.325840	-2.505898	2.529778
H	2.833146	-5.090176	-2.768394
H	4.147023	-1.599284	-2.850762
C	4.983785	-3.381080	-3.757909
C	2.625202	-2.538608	-4.065892
H	7.467610	2.128379	-1.294019
H	7.973772	1.858366	0.398005
H	8.004393	3.491529	-0.282173
H	6.456939	2.526286	2.297298
H	5.132371	3.677704	2.011006
H	6.818091	4.168277	1.702475
H	6.217871	4.830278	-0.657412
H	4.528755	4.353625	-0.377065
H	5.418875	3.668036	-1.749568
H	2.124461	3.978284	3.805747
C	1.584770	4.893888	1.943597
H	1.086511	5.484973	-0.055620
H	2.906977	2.836370	-1.919268
C	0.776084	3.217660	-2.005019
C	2.585782	4.939304	-2.321826
H	2.000853	-6.221446	-0.727660
H	4.766336	-3.115133	2.714296
H	3.440041	-4.194453	3.203370
H	3.637017	-2.612546	3.991745

H	1.303536	-2.019890	3.513054
H	0.952975	-3.528902	2.645994
H	0.644847	-1.956175	1.875130
H	4.675457	-4.404284	-4.004295
H	5.860851	-3.433435	-3.107319
H	5.270418	-2.876081	-4.689426
H	2.906083	-1.956021	-4.951592
H	1.767736	-2.056853	-3.592900
H	2.330375	-3.545493	-4.385853
H	1.046374	5.713471	2.408681
H	0.073320	4.017171	-1.747949
H	0.434320	2.309870	-1.499979
H	0.735995	3.050333	-3.089190
H	2.542663	4.774915	-3.405833
H	3.587709	5.293456	-2.062107
H	1.862600	5.725599	-2.075678

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