Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

All-Zinc Coordinated Nickel-Complexes as Molecular Mimics for NiZn Catalyst Surfaces, a Density Functional Theory Study

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Content

Computational Details:

Structures of the calculated molecules were optimized using the ORCA4.0[1] software package and Becke's exchange functional[2] with Perdew's correlation functional[3] (BP86). Grimme's Dispersion correction including Becke-Johnson damping (D3BJ)[4, 5] was used. After preoptimization and analytical calculation of the Hessian using Ahlrich's def2-SVP basis set, these structures were further optimized using the def2-TZVPP basis sets.[6] Frequency calculations were also performed on this level of theory showing no imaginary frequencies for most cases with the only exception being [Ni(ZnCp*)(ZnMe)(C_2H_4)$_3$] (rotation of the Me group at Zn). The resolution of identity approximation (RI) was applied to speed up the calculations.[7] Wiberg indices and NBO charges were computed using the NBO 3.1[8] program as implemented in Gaussian 09[9] program package with single point calculations (BP86/def2-TZVPP). Calculations within the Quantum Theory of Atom in Molecules (QTAIM) were performed using the MULTIWFN package[10], using Gaussian 09 .wfx files (BP86/def2-TZVPP). Energy Decomposition Analyses with the natural orbital for chemical valence extension (EDA-NOCV)[11-13] were carried out using the ADF (2013.01) program package[14] at the BP86/TZ2P+ level of theory with the previously optimized uncontracted Slater-type orbitals (STOs) were employed as basis functions in self-consistent field (SCF) calculations.[15] Triple-zeta quality basis sets were used which were augmented by two sets of polarization functions (p and d functions for H, d and f for other atoms). An auxiliary set of s, p, d, f and g STOs was used to fit the molecular densities and to represent the Coulomb and exchange potentials accurately in each SCF cycle. Scalar relativistic effects were considered using the zero-order regular approximation (ZORA).[16, 17, 18-20] The bond formation between the interacting fragments is divided into three steps within the EDA calculations. In the first step, these fragments (in the frozen geometry of the whole molecule) are superimposed without electronic relaxation yielding the quasi classical electrostatic attraction ΔE_{elstat}. The second step involves anti-symmetrization and normalization of the product wave function which gives the repulsive term ΔE_{Pauli}. In the final step, the molecular orbitals are allowed to relax which gives the stabilizing orbital interaction ΔE_{orb}. This orbital term can be further divided into contributions of different symmetry, representing different bonding situations (σ, π, etc.). Dispersion forces are accounted for using Grimme's D3 dispersion corrections. These contributions sum up to the total interaction energy ΔE_{int} :

$$\Delta E_{int} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{orb} + \Delta E_{disp}$$

Molecular structures

$[Ni(C_2Hx)_3]$

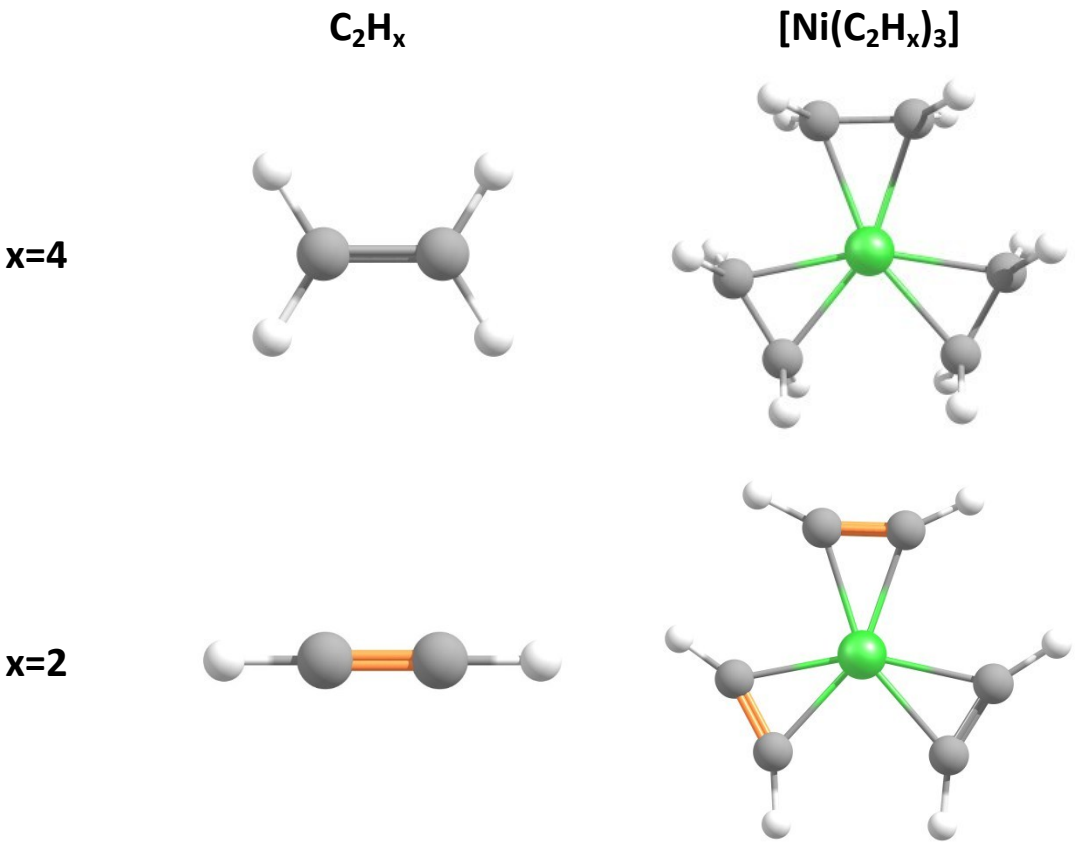


Figure S 1: Optimized Molecular structures (BP86-D3/def2-TZVPP) of C_2H_x and the parent $[Ni(C_2H_x)_3]$ complexes.

Table S 1: Summary of selected structural parameters of optimized C_2H_x and $[Ni(C_2H_x)_3]$ (BP86-D3/def2-TZVPP).

	Free ligands		$[Ni(C_2H_x)_3]$	
UHC	C_2H_4	C_2H_2	C_2H_4	C_2H_2
d(CC) [Å]	1.33	1.20	1.39	1.25
d(NiC) [Å]			2.05	1.99

Table S 2: Literature values for calculated structures of $[Ni(C_2H_x)_3]$ (x = 2,4).

$[Ni(C_2H_x)_3]$		
UHC	C_2H_4[21]	C_2H_2[22]
	(ZORA-BP86/TZ2P)	(B3LYP/SDD(Ni),631G(d)
d(CC) [Å]	1.394	1.248
d(NiC) [Å]	2.043	1.992

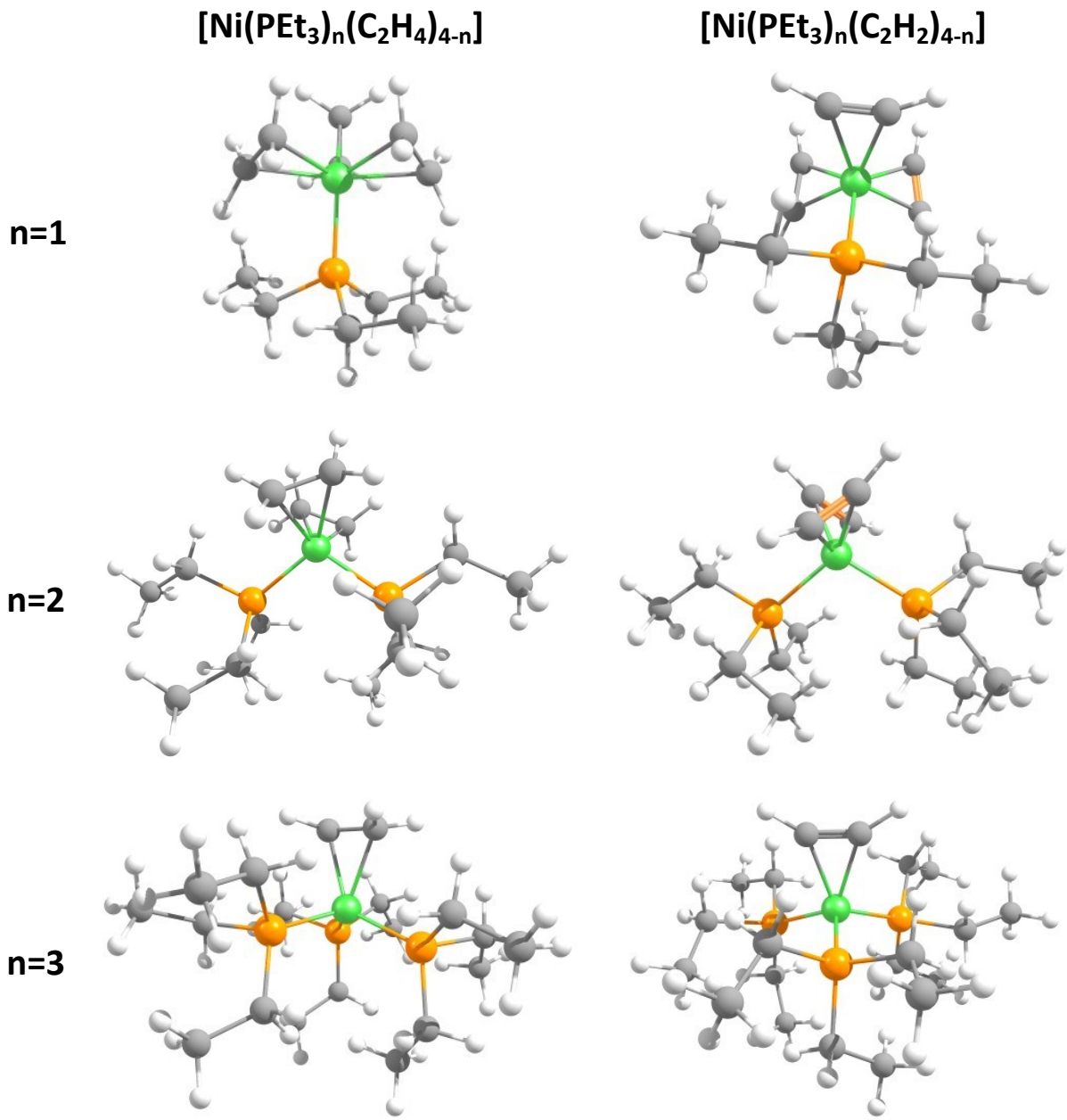


Figure S 2: Optimized Molecular structures (BP86-D3/def2-TZVPP) of $[Ni(PEt_3)_n(C_2H_x)_{4-n}]$.

Table S 3: Summary of selected structural parameters of optimized $[Ni(PEt_3)_n(C_2H_x)_{4-n}]$ (BP86-D3/def2-TZVPP).

	$[Ni(PEt_3)(C_2H_x)_3]$		$[Ni(PEt_3)_2(C_2H_x)_2]$		$[Ni(PEt_3)_3(C_2H_x)]$	
	C_2H_4	C_2H_2	C_2H_4	C_2H_2	C_2H_4	C_2H_2
d(C-C) [Å]	1.39	1.25	1.40	1.26	1.40	1.27
d(Ni-C) [Å]	2.08 - 2.12	2.02 - 2.10	2.08	1.91 - 2.04	2.06	2.00
d(Ni-P) [Å]	2.21	2.21	2.17	2.21	2.15-2.19	2.15-2.24
d(P-C) [Å]	<3.16	<3.15	<3.09	<3.11	<3.02	<3.06

$[Ni(ZnR)_{2n}(C_2H_x)_{4-n}]$

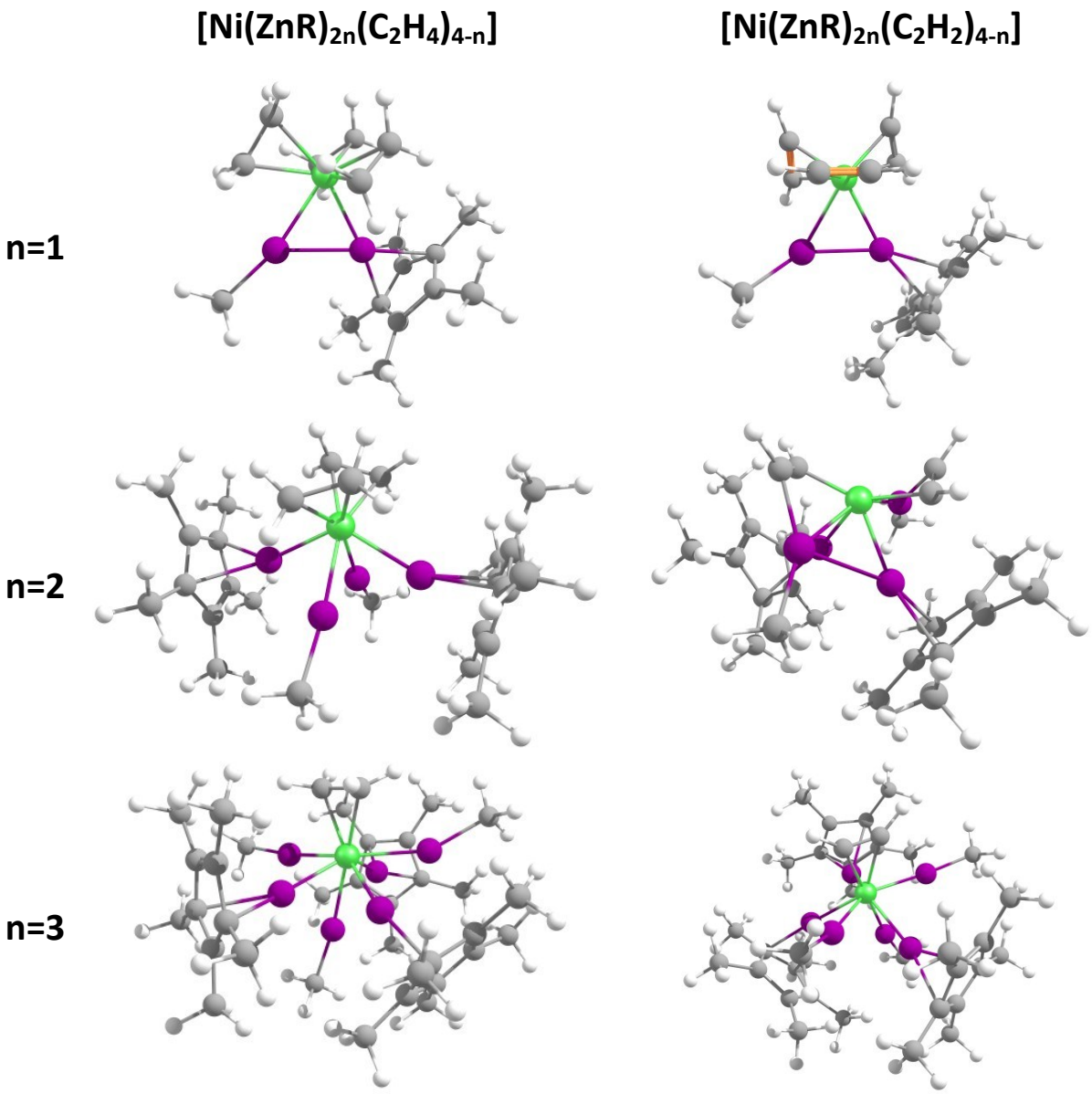
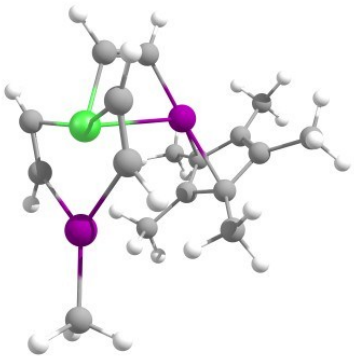


Figure S 3: Optimized Molecular structures (BP86-D3/def2-TZVPP) of $[Ni(ZnCp^*)_n(ZnMe)_n(C_2H_x)_{4-n}]$.

Table S 4: Summary of selected structural parameters of optimized $[Ni(ZnCp^*)_n(ZnMe)_n(C_2H_x)_{4-n}]$ (BP86-D3/def2-TZVPP).

	$[Ni(ZnCp^*)(ZnMe)(C_2H_x)_3]$		$[Ni(ZnCp^*)_2(ZnMe)_2(C_2H_x)_2]$		$[Ni(ZnCp^*)_3(ZnMe)_3(C_2H_x)]$	
	C_2H_4	C_2H_2	C_2H_4	C_2H_2	C_2H_4	C_2H_2
d(C-C) [Å]	1.40	1.25	1.40	1.34	1.42	1.28
d(Ni-C) [Å]	2.04 - 2.15	1.99 - 2.12	2.08	1.90 - 2.25	2.05	1.99
d(Ni-ZnR) [Å]	2.40	2.41	2.35	2.30 - 2.43	2.33 - 2.38	2.31 - 2.39
d(Zn-C) [Å]	> 2.41	> 2.76	>2.95	2.03	>2.57	>2.55
d(Zn-Zn) [Å]	2.46	2.45	> 2.62	> 2.72	>2.61	>2.59

Ni-Zn bridging output structure of $[Ni(ZnR)_2(C_2H_2)_3]$ (local minimum BP86-D3/def2-TZVPP):



	$[Ni(ZnCp^*)(ZnMe)(C_2H_2)_3]$	
	Non-bridging	bridging
d(C-C) [Å]	1.25	1.29-1.33
d(Ni-C) [Å]	1.99 - 2.12	1.87-2.75
d(Ni-ZnR) [Å]	2.41	2.38-3.05
d(Zn-C) [Å]	> 2.76	1.93-2.27
d(Zn-Zn) [Å]	2.45	4.20

This structure was obtained when C_2H_2 was put into Ni-Zn bridging coordinations before geometry optimization. Both $[Ni(ZnR)_2(C_2H_2)_3]$ structures are local minima on the potential energy surface. This minimum is about 15kcal/mol more stable. However, the Ni-Zn as well as Zn-Zn distances exceed standard distances.[23] Therefore, this structure was only included in the SI. The values discussed in the manuscript belong to the $[Ni(ZnR)_2(C_2H_2)_3]$ structure with non-bridging C_2H_2 ligands.

$[Ni(AlCp^*)_n(C_2H_x)_{4-n}]$

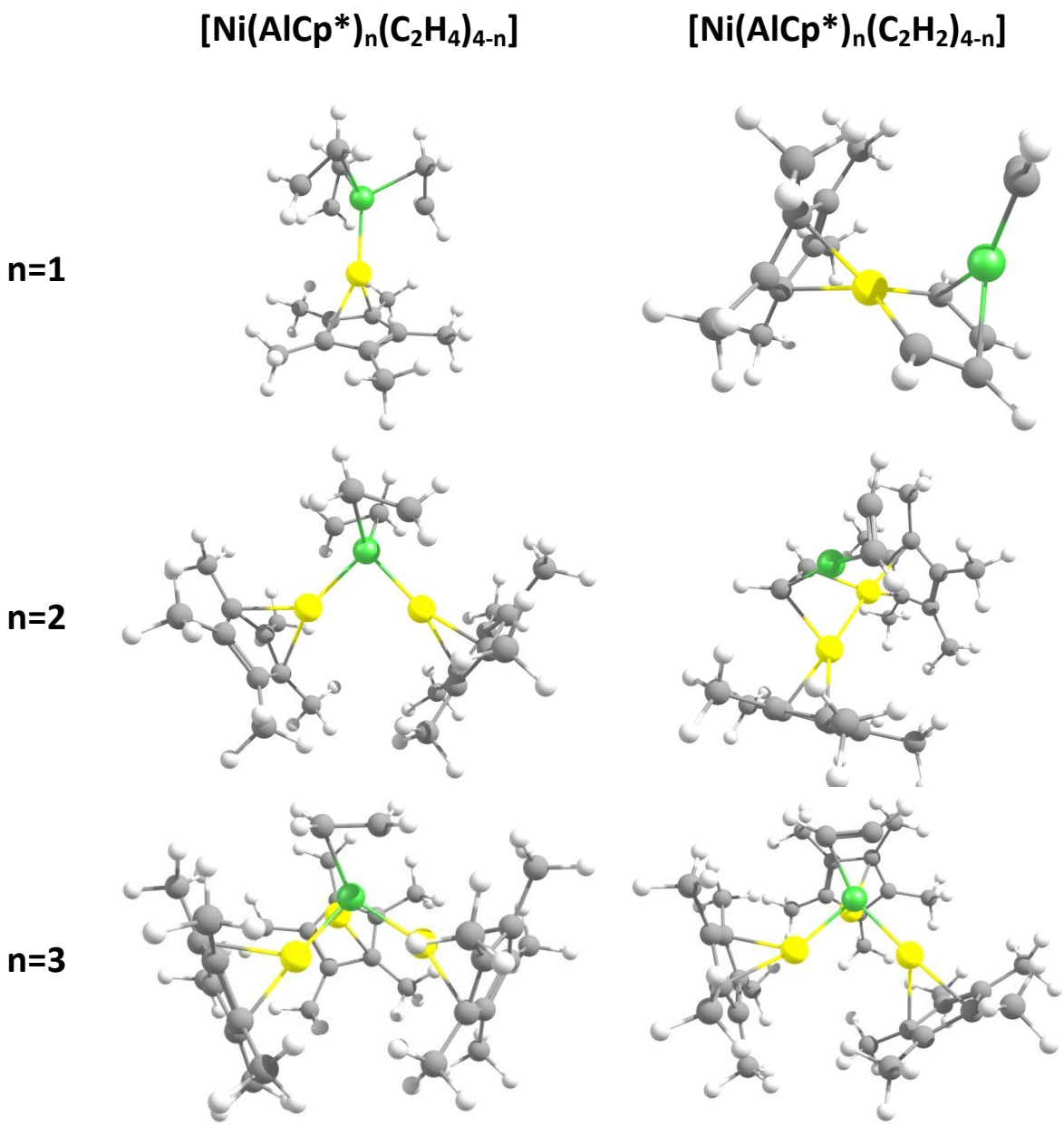


Figure S 4: Optimized Molecular structures (BP86-D3/def2-TZVPP) of $[Ni(AlCp^*)_n(C_2H_x)_{4-n}]$.

Table S 5: Summary of selected structural parameters of optimized $[Ni(AlCp^*)_n(C_2H_x)_{4-n}]$ (BP86-D3/def2-TZVPP).

	$[Ni(AlCp^*)(C_2H_x)_3]$		$[Ni(AlCp^*)_2(C_2H_x)_2]$		$[Ni(AlCp^*)_3(C_2H_x)]$	
	C_2H_4	C_2H_2	C_2H_4	C_2H_2	C_2H_4	C_2H_2
d(C-C) [Å]	1.39-1.40	1.28-1.47	1.41	1.27-1.37	1.41	1.27
d(Ni-C) [Å]	2.05-2.17	1.86-2.17	2.05-2.07	1.88-2.24	2.03	1.94
d(Ni-AlCp*) [Å]	2.25	2.48	2.21	2.45-2.60	2.20-2.23	2.22-2.27
d(Al-C) [Å]	> 2.97	1.98	> 3.01	2.04-2.18	> 3.18	> 3.24
d(Al-Al) [Å]			3.12	2.50	3.25	> 3.21

$[Ni(GaCp^*)_n(C_2H_x)_{4-n}]$

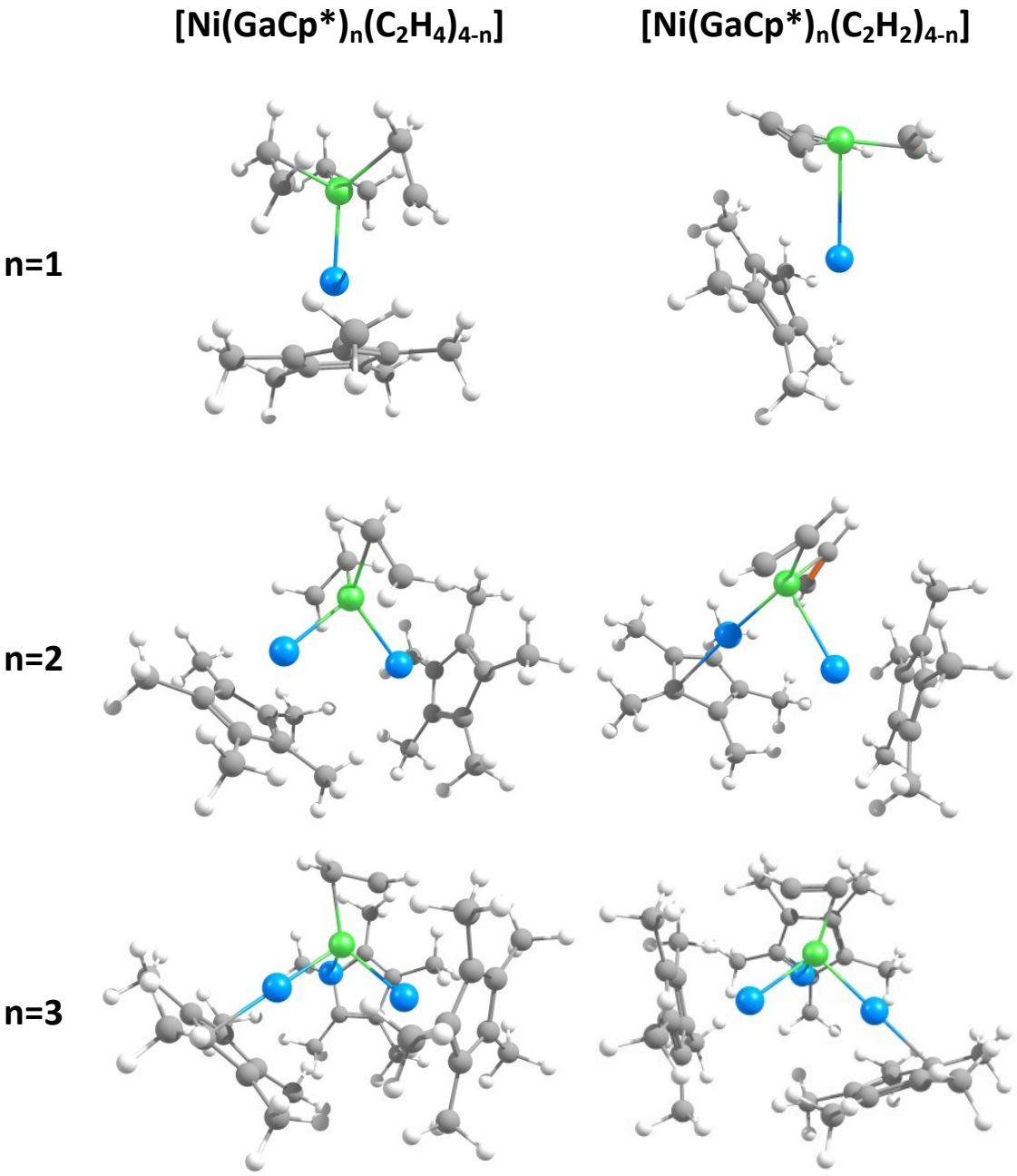


Figure S 5: Optimized Molecular structures (BP86-D3/def2-TZVPP) of $[Ni(GaCp^*)_n(C_2H_x)_{4-n}]$.

Table S 6: Summary of selected structural parameters of optimized $[Ni(AlCp^*)_n(C_2H_x)_{4-n}]$ (BP86-D3/def2-TZVPP).

	$[Ni(GaCp^*)(C_2H_x)_3]$		$[Ni(GaCp^*)_2(C_2H_x)_2]$		$[Ni(GaCp^*)_3(C_2H_x)]$	
	C_2H_4	C_2H_2	C_2H_4	C_2H_2	C_2H_4	C_2H_2
d(C-C) [Å]	1.39	1.25	1.40	1.26	1.40	1.27
d(Ni-C) [Å]	2.06-2.14	1.98-2.00	2.02-2.08	1.95-1.97	2.02-2.03	1.93
d(Ni-GaCp*) [Å]	2.37	3.21	2.34-2.37	2.29, 2.70	2.273-2.325	2.28-2.40
d(Ga-C) [Å]	>3.10	>3.58	>3.10	>3.02	>3.10	>3.27
d(Ga-Ga) [Å]			3.39	3.31	>3.39	>3.32

NBO, WBI QTAIM and EDA-NOCV Results:

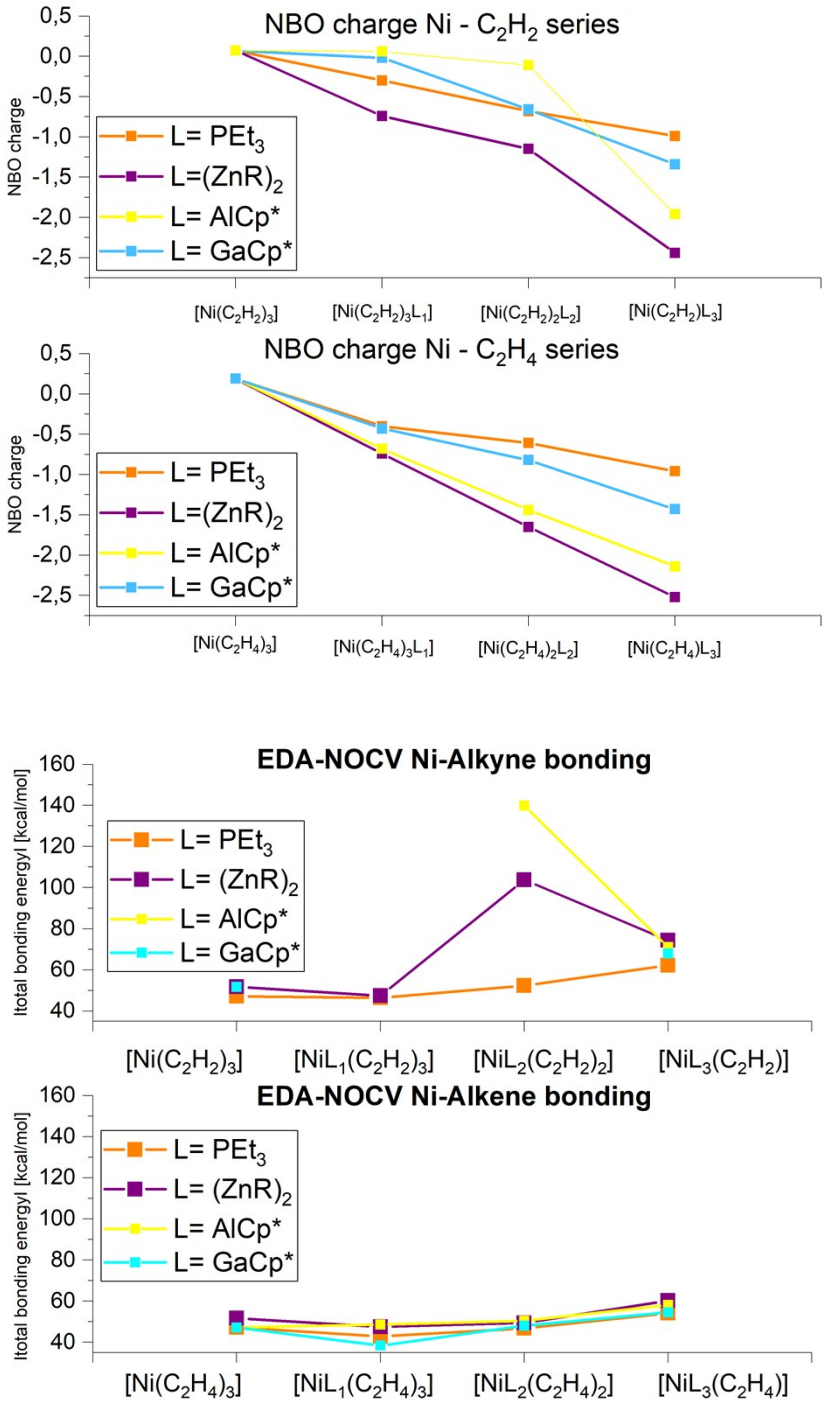


Figure S 6: Top: NBO charges calculated for Ni in [Ni(L)$_n$(C_2H_x)$_{4-n}$] (L = PEt_3, AlCp*; GaCp*, $(ZnR)_2$) Bottom: Results of the EDA-NOCV calculations showing the ΔE_{int} values obtained for (C2Hx) interaction to the respective [NiL$_n$(C_2H_x)$_m$] fragment.

From parent [Ni(C_2H_x)$_3$] to [Ni(PEt_3)$_n$(C_2H_x)$_{4-n}$] without P-C_2H_x interaction, ΔE_{int} marginally decreases for [Ni(PEt_3)$_1$(C_2H_x)$_3$] before it increases with higher numbers of coordinated PEt_3. As expected, ΔE_{int} is slightly higher for the alkyne series compared to the alkene series, due to higher Ni->C_2H_x π-back and C_2H_x->Ni σ contributions in the orbital share. The general trend in the Ni-C_2H_x total interaction energy is independent of L, i.e. ZnR vs. PEt_3. $(ZnR)_{2n}$ coordination leads to a slightly higher value of ΔE_{int} compared to PEt_3 coordination due to higher

electrostatic and covalent contributions. Again, the $NiZn_4$ acetylene complex $[Ni(ZnR)_4(C_2H_2)_2]$ is a special case. Here, ΔE_{int} is by far higher than for any other member of the series. When taking a closer look at the electrostatic and covalent contributions to ΔE_{int}, a significant feature becomes evident for the $NiZn_4$ environment. In the side-on coordinated C_2H_x in $[Ni(PEt_3)_n(C_2H_x)_{4-n}]$ and $[Ni(ZnR)_{2n}(C_2H_x)_{4-n}]$ (except $[Ni(ZnR)_4(C_2H_2)_2]$) the Ni-C_2H_x bond is dominated by electrostatic interactions. This situation changes for $[Ni(ZnR)_4(C_2H_2)_2]$. Here the covalent contribution slightly exceeds the electrostatic interaction. The preparation energy ΔE_{Prep} which summarizes the necessary energy to distord the respective fragments from its relaxed geometry to the geometry in respective compound is also given in Table S7. As evident from the respective structures of the alkyne compounds $[Ni(ER)_2(C_2H_2)_2]$ (E= Al, Zn) , the preparation energy is largest for E= Al, Zn. For both compounds, the alkyne as well as the $N(ER)_2$ fragment require about the same preparation energy (data not shown), which also points to significant alkyne activation within these compounds. The preparation energy together with the interaction energy yield the bonding interaction ΔE. Taking these values into account the ΔE values are in the same range of about 20kcal/mol for the C_2H_2 and C_2H_4 - $Ni(ER)_2$ interaction.

Table S 7: Overwiev of EDA-NOCV results for $[NiL_2(C_2H_x)_2]$ (L = PEt_3, AlCp*, $(ZnR)_2$) and the respective WBI values of the C-C bonds showing distinct C_2H_x bonding on NiL_2 fragments.

	$[NiL_2(C_2H_4)_2]$			$[NiL_2(C_2H_2)_2]$		
L=	PEt_3	$(ZnR)_2$	AlCp*	PEt_3	$(ZnR)_2$	AlCp*
ΔE_{int} [kcal/mol]	-46.8	-49.4	-50.5	-52.4	-103.8	-139.9
ΔE_{Pauli} [kcal/mol]	171.4	177.0	169.3	181.2	348.3	379.7
$\Delta E_{electrostat}$ [kcal/mol]	-122.5	-123.6	-121.4	-126.9	-215.7	-235.3
ΔE_{orb} [kcal/mol]	-85.7	-89.5	-89.6	-97.9	-225.0	-275.4
π-type interaction [kcal/mol]	-54.9	-48.8	-55.8	-63.6		
σ-type interaction [kcal/mol]	-20.8	-27.6	-23.3	-23.1		
ΔE_{Disp} [kcal/mol]	-9.9	-13.4	-8.8	-8.8	-11.22	-8.8
ΔE_{Prep} [kcal/mol]	11.0	28.3	28.0	10.3	90.6	109.65
WBI (C-C)	1.51	1.48	1.45	2.43	1.93	1.76

	[Ni(C_2H_x)$_3$]		[Ni(L)(C_2H_x)$_3$]		[Ni(L)$_2$(C_2H_x)$_2$]		[Ni(L)$_3$(C_2H_x)]			
NBO charges	C_2H_4	C_2H_2	C_2H_4	C_2H_2	C_2H_4	C_2H_2	C_2H_4	C_2H_2	C_2H_4	C_2H_2
Ni			0.19	0.07	-0.74 (-0.30)	-0.74 (-0.40)	-1.65 (-0.61)	-1.15 (-0.68)	-2.52 (-0.96)	-2.44 (-0.99)
Zn					0.94	0.90	0.90 - 0.95	0.95 - 1.08	0.79 - 1.06	0.75 - 1.08
C	-0.39	-0.24	-0.47	-0.25	-0.42 - -0.57 (-0.45)	-0.19 - -0.30 (-0.24)	-0.41 (-0.47)	-0.28 (Ni); -0.64 (Zn) (-0.25 - -0.28)	-0.44 (-0.47)	-0.26 (-0.28)
Wiberg bond index (CC)	2.05	3.00	1.53	2.43	1.49 (1.55)	2.38 - 2.46 (2.45 - 2.50)	1.48 (1.51)	1.93 (2.43)	1.38 (1.48)	2.21 (2.37)

Table S 8: Summary of NBO and WBI results for all compounds. Values in parenthesis refer to [Ni(PEt_3)$_n$(C_2H_x)$_{4-n}$]. Values without parenthesis refer to [Ni($ZnCp^*$)$_n$($ZnMe$)$_n$(C_2H_x)$_{4-n}$].

Table S 9 Summary of EDA-NOCV results for all complexes. Values in parenthesis refer to [Ni(PEt_3)$_n$(C_2H_x)$_{4-n}$], values without parenthesis refer to [Ni($ZnCp^*$)$_n$($ZnMe$)$_n$(C_2H_x)$_{4-n}$]. The bonding interaction of one C_2H_x fragment with the remaining [Ni(L)$_n$(C_2H_x)$_{(4-(n+1))}$] fragment was investigated.

	[Ni(C_2H_x)$_3$]		[Ni(L)(C_2H_x)$_3$]		[Ni(L)$_2$(C_2H_x)$_2$]		[Ni(L)$_3$(C_2H_x)]	
	C_2H_4	C_2H_2	C_2H_4	C_2H_2	C_2H_4	C_2H_2	C_2H_4	C_2H_2
Total Bonding Energy [kcal/mol]	-47.2	-51.7	-47.5 (-42.9)	-47.4 (-46.4)	-49.4 (-46.8)	-103.8 (-52.4)	-60.3 (-54.2)	-74.3 (-62.2)
Total Pauli Repulsion [kcal/mol]	130.74	134.6	191.8 (146.1)	208.6 (180.8)	177.0 (171.4)	348.3 (181.2)	181.6 (177.1)	197.7 (181.6)
Total Electrostatic Interaction [kcal/mol]	-99.5	-101.58	-132.3 (-103.9)	-140.9 (-126.2)	-123.6 (-122.5)	-215.7 (-126.9)	-128.8 (-126.7)	-137.4 (-128.9)
Total Orbital Interaction [kcal/mol]	-73.2	-80.17	-97.4 (-74.4)	-105.1 (-91.9)	-89.5 (-85.7)	-225.0 (-97.9)	-98.5 (-92.9)	-121.5 (-104.7)
π-type interaction	-41.9	-47.3	-56.3 (-42.1)	-58.5 (-56.6)	-48.8 (-54.9)	(-63.6)	-53.4 (-59.63)	-71.6 (-70.7)
σ_{back}-type interaction	-22.5	-22.0	-28.0 (-21.9)	-31.5 (-24.5)	-27.6 (-20.8)	(-23.08)	-30.3 (-21.26)	-31.1 (-21.5)

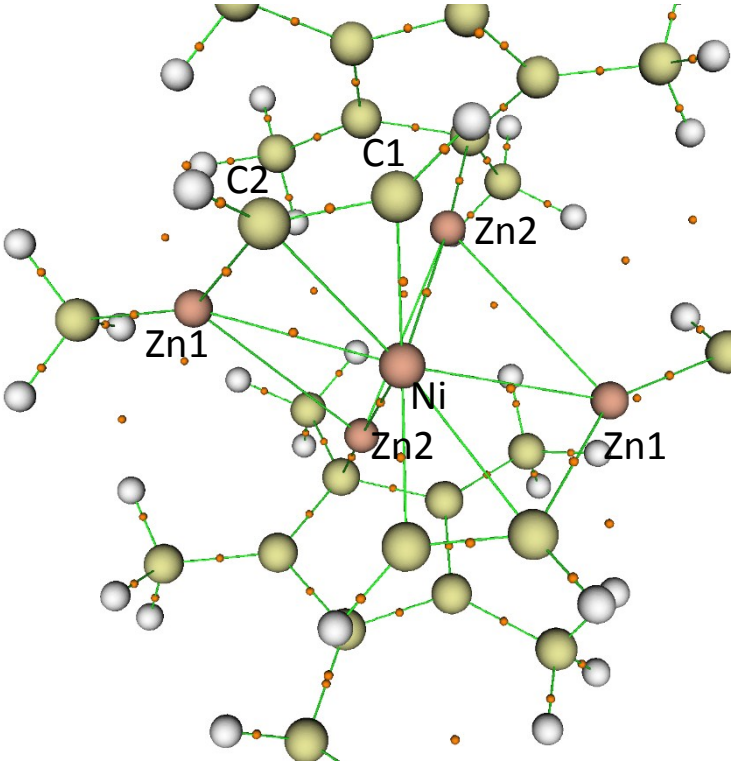


Figure S 7: QTAIM results showing bond paths (green) and bond critical points (orange dots) for $[Ni(ZnR)_4(C_2H_2)_2]$ showing Ni-Zn bonding interactions for all NiZn interactions.

Preliminary experimental results:

Synthetic protocols.

Proofs for reductive elimination of H-$SiEt_3$ from [(H)($SiEt_3$)NiL_n] complexes (L = AlCp*, ZnR) as a potential approach to attach unsaturated hydrocarbons to [NiL_n] fragments.

[(H)($SiEt_3$)Ni(AlCp*)$_3$][24]. [Ni(cod)$_2$] (204 mg, 0.74 mmol, 1.0 eq.) and AlCp* (355 mg, 2.19 mmol, 3.0 eq.) was suspended in triethylsilane (5 mL) and heated to 75 °C for 3 hours. The mixture was cooled to ambient temperature and all volatiles were removed in vacuo. The brownish residue was washed with hexane (2.5 mL), filtered and dried under vacuo. The solid was *Whatman*-filtered with boiling hexane (8 mL, removal of residual AlCp*). The filtrate was dried to obtain a yellowish brown powder of AlCp* free [(H)($SiEt_3$)Ni(AlCp*)$_3$]. Yield: 200 mg, (0.30 mmol, 41%). ^{1}H NMR (400 MHz, 298 K, C_6D_6): δ (ppm) = 1.89 (s, 45 H), 1.27 (t, ^3J = 7.8 Hz, 9 H), 0.85 (q, ^3J = 7.8 Hz, 6 H), -12.79 (s, 1 H).

[Ni(PEt_3)(AlCp*)$_3$][25]. A sample of [(H)($SiEt_3$)Ni(AlCp*)$_3$] (200 mg, 0.30 mmol, 1 eq.) was suspended in 5 mL n-hexane and a sample of PEt_3 (0.087 ml, 0.60 mmol, 2 eq.) was added. The yellow suspension was stirred at 60 °C for 1.5 h. After cooling to room temperature, all volatile components were removed *in vacuo* resulting in a yellow solid, which was re-crystallized, from cold n-hexane (2 mL). The solvent was removed with a cannula, the remaining yellow crystalline solid was dried. Yield: 133 mg (0.20 mmol, 65%). ^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 1.98 (s, 45H), 1.05 (m, 6H), 0.99 (m, 9H) ppm; ^{13}C-NMR (100.6 MHz, C_6D_6, 298K): δ = 112.8 (s, C_5Me_5) , 29.0 (d, J=17.7 Hz, CH_2), 10.4 (d, J=4.9 Hz, CH_3) 10.3 (s, C_5Me_5) ppm; ^{27}Al-NMR (104.6 MHz, C_6D_6, 298K): δ = -53.1(s) ppm; ^{31}P-NMR (162.0 MHz, C_6D_6, 298K): δ = 61.9 (s) ppm; IR (cm^{-1}): 2949, 2911, 2860, 1451, 1426, 1375, 1258, 1023, 800, 762, 722, 662, 620, 584, 560, 599, 453, 440. Elemental anal. calcd for $C_{36}H_{60}$Al3NiP: C, 65.17; H, 9.12; Al, 12.20; P, 4.67; Ni, 8.85, found: C, 64.75; H, 9,01; Al, 12.0; P, 4.41; Ni, 8.3.

[(H)($SiEt_3$)Ni($ZnCp^*$)$_2$($ZnMe$)$_2$(AlCp*)] (to be published). $ZnMe_2$ (77 mg, 0.807 mmol, 5.3 eq.) was added dropwise as a solution in toluene (5 mL) with a cooled (-50 °C) addition funnel to a solution of [Ni(AlCp*)$_3$(H)($SiEt_3$)] (100 mg, 0.151 mmol, 1.0 eq.) in toluene (3 mL) over 15 min. After stirring for 3 h at -50 °C, the mixture was concentrated for 1 h to reach about 50% of the volume (at -50°C). The volatiles were removed under vacuo while the mixture was allowed to reach r.t. to obtain a dark green residue. ^{1}H NMR (400 MHz, 298 K, C_6D_6): δ (ppm) = 2.18 (s, 30 H, H_{ZnCp^*}), 1.76 (s, 15 H, H_{AlCp^*}), 1.07 (t, ^3J = 7.8 Hz, 9 H, H_{SiEt3}), 0.70 (q, ^3J = 7.7 Hz, 6 H, H_{SiEt3}), -0.10 (s, 6 H, H_{ZnMe}), -12.0 (s, 1 H, H_{Ni-H}). LIFDI MS (toluene): [M]$^+$: 898.56 (calculated: 898.13).

[(PEt_3)Ni($ZnCp^*$)$_2$($ZnMe$)$_2$($AlCp^*$)] (to be published). PEt_3 (77 mg, 0.807 mmol, 5.3 eq.) was added to a solution of [Ni($AlCp^*$)$_1$($ZnCp^*$)$_2$($ZnMe$)$_2$(H)($SiEt_3$)] (100 mg, 0.151 mmol, 1.0 eq.) in C_6D_6 and heated to 80°C for 5 min. ^{1}H NMR (400 MHz, 298 K, C_6D_6): δ (ppm) = 2.24 (s, 30 H, H_{ZnCp^*}), 1.80 (s, 15 H, H_{AlCp^*}), 1.42 (m, 6 H, H_{PEt3}), 0.80 (m, 9 H, H_{PiEt3}), -0.08 (s, 6 H, H_{ZnMe}). ^{31}P NMR (162 MHz, 298 K, C_6D_6): 46.4 ppm.

XYZ-coordinates:

$[Ni(PEt_3)(C_2H_4)_3]$:

Ni	-0.440397	-0.080555	-0.225277
P	-2.630312	0.183735	-0.342301
C	-3.138492	-1.033940	-2.929598
C	-3.468615	0.136883	-2.004921
C	-2.763578	3.044876	-0.409166
C	-3.355374	1.796769	0.244537
C	-3.440652	-2.427527	0.581490
C	-3.712879	-0.927122	0.692227
C	0.029998	1.103013	-1.919593
C	1.197384	0.612807	-1.341368
C	-0.166658	1.344879	1.268591
C	0.318603	0.121196	1.720730
C	0.301005	-2.032738	0.015044
C	-0.415661	-1.945039	-1.173366
H	-2.062885	-1.083929	-3.134002
H	-3.660878	-0.922065	-3.890135
H	-3.442000	-1.997775	-2.501054
H	-3.175305	1.076493	-2.496970
H	-4.554890	0.200060	-1.828134
H	-1.684450	3.111145	-0.225944
H	-3.233948	3.954327	-0.010305
H	-2.916284	3.045872	-1.496720
H	-3.206331	1.832786	1.334187
H	-4.444799	1.752658	0.083570
H	-3.642034	-2.808118	-0.428226
H	-4.078873	-2.990373	1.276925
H	-2.395979	-2.657602	0.824939
H	-4.767413	-0.701349	0.462182
H	-3.540239	-0.599921	1.729871
H	-0.284109	2.131923	-1.749209
H	-0.389862	0.632065	-2.808811
H	1.815959	1.247456	-0.705533
H	1.710288	-0.251514	-1.765766
H	-1.116206	1.725287	1.640617
H	0.512537	2.106605	0.883551
H	-0.265525	-0.482756	2.415013
H	1.384958	-0.099196	1.694351
H	-0.136297	-2.512853	0.890321
H	1.388055	-1.963767	0.019721
H	-1.405909	-2.387235	-1.247251
H	0.097120	-1.804298	-2.125853

$[Ni(PEt_3)(C_2H_2)_3]$:

Ni	-0.508432	-0.080146	-0.237149
P	-2.697611	0.199964	-0.374937
C	-0.380614	-2.049586	-0.972550
C	0.667356	-1.776313	-0.354879
C	-0.397152	-0.142158	1.784073
C	-0.163997	1.038182	1.429598
C	0.935669	0.969710	-1.279035
C	-0.098520	1.001629	-1.975774
C	-3.717549	-0.868775	0.744921
C	-3.494826	-2.371480	0.571183
C	-3.256271	1.860162	0.230367
C	-2.615897	3.030859	-0.516286
C	-3.578475	0.104300	-2.005564
C	-3.124289	-1.040278	-2.913021
H	1.643000	-1.919948	0.076628
H	-1.047714	-2.664033	-1.549788
H	1.955103	1.161812	-0.992256
H	-0.695770	1.265396	-2.831274
H	-0.494772	-0.959237	2.481564
H	0.097599	2.074367	1.574697
H	-3.424542	-0.564258	1.762021
H	-4.780386	-0.603106	0.624695
H	-2.428943	-2.617508	0.664070
H	-4.048026	-2.940847	1.331043
H	-3.834009	-2.721718	-0.412914
H	-4.356421	1.912331	0.191806
H	-2.967534	1.888748	1.291972
H	-2.929969	3.064080	-1.568904
H	-2.899031	3.989847	-0.060829
H	-1.521308	2.948377	-0.501447
H	-4.663241	0.062872	-1.818040
H	-3.384404	1.066085	-2.504323
H	-3.364652	-2.020752	-2.481656
H	-3.613932	-0.981653	-3.895067
H	-2.037704	-1.003359	-3.065694

$[Ni(PEt_3)_2(C_2H_4)_2]$:

Ni	-0.172959	3.607152	4.339062
P	0.037126	2.482119	2.494919
P	-0.128507	2.177786	5.975297
C	1.113776	5.129552	3.765510
C	1.559777	4.572973	4.970766
C	-1.645979	4.851303	5.098386
C	-2.000100	4.440215	3.807430
C	-2.873898	1.550728	6.164617
C	-0.393193	2.108992	8.884932
C	1.503689	-0.049790	5.197928
C	2.077015	0.750937	1.252417
C	0.062165	3.065040	-0.394898
C	-1.353778	0.297318	1.059593
C	-0.167742	2.988211	7.654119
C	1.369399	1.094246	6.202695
C	-0.493548	3.433605	0.983185
C	-0.964384	0.912454	2.406232
C	1.796946	2.000495	2.090147
C	-1.484278	0.913384	6.122598
H	1.360655	5.078340	5.916635

H	0.549576	6.064208	3.760171
H	1.643605	4.917317	2.835231
H	2.424589	3.906623	4.977947
H	-1.851491	5.107739	2.957799
H	-1.207613	5.836897	5.267151
H	-2.158903	4.429793	5.963279
H	-2.777432	3.686960	3.662514
H	0.350524	1.304316	8.965136
H	-1.386907	1.641563	8.873091
H	-0.324356	2.707100	9.804930
H	-3.037921	2.183429	5.282504
H	-3.001293	2.185931	7.052191
H	-3.66278 0	0.786238	6.188260
H	1.486687	0.318865	4.165747
H	0.690390	-0.779718	5.306110
H	2.450627	-0.588851	5.340761
H	-0.210859	2.048347	-0.700029
H	1.157608	3.138299	-0.418111
H	-0.324238	3.755592	-1.158877
H	1.667271	0.832414	0.238803
H	1.645431	-0.146760	1.715909
H	3.160055	0.581949	1.161591
H	-0.480431	-0.012973	0.474433
H	-1.934269	1.002845	0.451154
H	-1.982176	-0.592046	1.214895
H	-1.399421	0.265873	5.238757
H	-1.312566	0.275054	7.003780
H	0.792465	3.521248	7.726196
H	-0.934237	3.772713	7.598460
H	2.235190	1.769012	6.130806
H	1.364169	0.688263	7.225678
H	2.238490	2.890575	1.615423
H	2.298081	1.917554	3.064780
H	-1.593759	3.398478	0.985113
H	-0.234654	4.475909	1.219181
H	-0.426233	0.180449	3.026611
H	-1.873318	1.162552	2.973542

$[Ni(PEt_3)_2(C_2H_2)_2]$:

Ni	0.084059	3.527512	4.391915
P	-0.159100	2.120194	6.071476
P	0.057724	2.387866	2.497922
C	-1.503779	0.837788	6.040816
C	1.770844	2.046331	1.853906
C	-0.830312	0.751859	2.472098
C	-0.746679	3.358494	1.127177
C	1.291369	1.070670	6.553405
C	-0.513967	3.018631	7.656626
C	-1.339584	0.149672	1.159808
C	-0.357893	3.097845	-0.330296
C	2.017902	0.856794	0.925772
C	1.844115	0.253215	5.385691
C	-0.768753	2.199526	8.922306
C	-2.877700	1.445383	5.753882
C	-1.700738	4.484895	4.167900
C	-1.059805	5.053798	5.089281
C	2.024437	3.993060	4.770539
C	1.600688	4.736439	3.844484
H	2.807900	3.693370	5.451186
H	1.700438	5.551978	3.142765
H	-0.886597	5.823152	5.825935
H	-2.566944	4.411429	3.527375
H	-1.679773	0.907825	3.152527
H	-0.161186	0.049860	2.993722
H	-0.539964	4.406505	1.389214
H	-1.831180	3.231209	1.271656
H	2.392968	1.958513	2.756342
H	2.099109	2.986411	1.385023
H	1.013053	0.413672	7.391586
H	2.060733	1.762398	6.928116
H	-1.370479	3.672007	7.432479
H	0.343261	3.696684	7.789142
H	-1.506417	0.274756	6.987286
H	-1.231432	0.123691	5.250647
H	-1.872514	-0.792909	1.353945
H	-2.046891	0.825379	0.661420
H	-0.528491	-0.067012	0.455617
H	3.089783	0.767261	0.695112
H	1.706562	-0.087388	1.392717
H	1.481600	0.952538	-0.025980
H	-0.889678	3.790866	-0.998795
H	0.717186	3.254461	-0.489948
H	-0.597324	2.077732	-0.652160
H	2.740335	-0.310280	5.680075
H	1.105351	-0.471720	5.016207
H	2.110940	0.913303	4.550290
H	-3.645624	0.666938	5.645042
H	-3.195230	2.118685	6.561757
H	-2.852024	2.043329	4.833002
H	-0.943223	2.859118	9.784602
H	-1.654326	1.557878	8.819555
H	0.083818	1.553380	9.171684

$[Ni(PEt_3)_3(C_2H_4)]$:

Ni	-0.436091	-0.210776	0.028325
P	0.035870	0.976972	1.786585
P	0.279933	0.647989	-1.864063
P	0.372305	-2.207266	0.118765
C	-2.356033	-0.931285	-0.202994
C	-2.382686	0.461907	-0.028104
C	3.140105	-1.630608	0.645592
C	2.193013	-2.569861	-0.096455
C	0.718669	-2.826454	2.883356
C	-0.043527	-3.231260	1.620797

C	-0.315651	0.586076	4.693137
C	-0.944714	0.449578	3.304646
C	2.663470	1.903218	1.440449
C	1.771226	1.159088	2.437048
C	2.754828	1.140305	-3.419374
C	2.008084	0.231914	-2.439543
C	0.050129	3.248062	-3.285460
C	0.207634	2.513557	-1.951147
C	-0.327462	3.656154	2.912187
C	-0.446155	2.777033	1.666581
C	-0.270896	0.144255	-4.738486
C	-0.794807	0.112883	-3.300443
C	0.276276	-4.732930	-1.374028
C	-0.296654	-3.322151	-1.223093
H	-2.551370	1.121957	-0.881894
H	-2.493600	-1.357835	-1.197877
H	-2.652203	-1.588264	0.617778
H	-2.717883	0.879274	0.923223
H	0.893885	3.075821	-3.963389
H	-0.025781	4.333273	-3.119097
H	-0.865928	2.935870	-3.804260
H	-0.017222	1.157679	-5.069948
H	-1.026373	-0.253161	-5.433066
H	0.627933	-0.477571	-4.848079
H	2.857448	2.156876	-3.016964
H	2.250635	1.213538	-4.389722
H	3.770891	0.758366	-3.599943
H	0.173465	-5.320748	-0.451678
H	1.341130	-4.716655	-1.640174
H	-0.251547	-5.281181	-2.167932
H	0.704351	-1.737734	3.023494
H	1.768924	-3.141866	2.834084
H	0.278778	-3.285368	3.779770
H	3.089373	-1.772060	1.732061
H	2.880106	-0.585532	0.442090
H	4.182697	-1.793230	0.337037
H	0.598542	-0.016698	4.780460
H	-1.012480	0.236536	5.469295
H	-0.049050	1.623589	4.930189
H	2.523471	1.513077	0.421548
H	3.726288	1.805052	1.700585
H	2.424817	2.975030	1.414809
H	-0.990054	3.309877	3.716339
H	-0.605277	4.696169	2.685657
H	0.697528	3.671108	3.308198
H	-1.481055	2.774427	1.295169
H	0.158833	3.187969	0.846220
H	-0.163311	-2.755526	-2.157384
H	-1.381804	-3.364105	-1.053628
H	2.373114	-2.488530	-1.179631
H	2.387906	-3.618516	0.176069
H	-1.125495	-3.095492	1.767757
H	0.122178	-4.298652	1.408643
H	-1.219233	-0.597820	3.121129
H	-1.888348	1.015288	3.254147
H	2.150756	0.142103	2.602957
H	1.780147	1.668028	3.411231
H	-1.090802	-0.915295	-3.044124
H	-1.718665	0.706433	-3.209392
H	2.590268	0.145978	-1.511519
H	1.940022	-0.794996	-2.833857
H	-0.638364	2.766478	-1.295842
H	1.104650	2.862008	-1.414329

$[Ni(PEt_3)_3(C_2H_2)]$:

Ni	-0.378820	-0.226727	-0.015794
P	0.415481	-2.224937	0.066804
P	0.355166	0.641953	-1.856920
P	0.088967	0.998675	1.799018
C	-0.323679	-3.288509	-1.274862
C	0.067367	-4.765243	-1.364606
C	-0.715184	0.120153	-3.298036
C	-0.167388	0.137060	-4.726603
C	-0.522655	2.757483	1.689778
C	-0.484323	3.636269	2.940429
C	0.279295	2.505674	-1.912742
C	0.129145	3.248323	-3.243252
C	2.088306	0.235155	-2.419641
C	2.836996	1.155451	-3.386666
C	1.813004	1.270151	2.447549
C	2.676948	2.002997	1.418461
C	-0.861606	0.398353	3.303097
C	-0.241847	0.554245	4.692797
C	0.019569	-3.238164	1.578034
C	0.811123	-2.836193	2.824617
C	2.225290	-2.604674	-0.184840
C	3.173639	-1.672265	0.570058
C	-2.284843	0.308890	-0.310586
C	-2.273873	-0.782666	0.332428
H	-2.852722	1.096342	-0.788661
H	-2.831495	-1.584886	0.797968
H	1.170633	2.851522	-1.365678
H	-0.573453	2.744580	-1.262132
H	2.028311	-0.788258	-2.823393
H	2.663446	0.145600	-1.488193
H	-1.624161	0.736310	-3.218601
H	-1.041819	-0.895776	-3.034212
H	1.810870	1.813064	3.403917
H	2.228588	0.271712	2.646384
H	-1.836026	0.907803	3.250787
H	-1.079824	-0.659690	3.104734
H	0.174200	-4.306598	1.366034
H	-1.057449	-3.093111	1.747055
H	2.423377	-3.657454	0.069513

H	2.393959	-2.504815	-1.268076
H	-1.412761	-3.172715	-1.167337
H	-0.064851	-2.769331	-2.210665
H	0.049319	3.223543	0.874785
H	-1.552879	2.662260	1.311813
H	0.534949	3.730434	3.340948
H	-0.844481	4.652553	2.720758
H	-1.119569	3.230454	3.738748
H	2.367379	3.051743	1.312098
H	3.737898	1.996351	1.703958
H	2.585904	1.533560	0.427911
H	-0.033563	1.602516	4.941686
H	-0.917125	0.157440	5.465563
H	0.705413	0.003571	4.774317
H	4.209083	-1.785839	0.219006
H	2.872371	-0.626596	0.431124
H	3.164493	-1.867239	1.649123
H	0.367882	-3.267081	3.733120
H	1.849436	-3.187211	2.767464
H	0.834439	-1.745660	2.947352
H	-0.430305	-5.247644	-2.218545
H	1.149612	-4.892927	-1.501642
H	-0.222301	-5.322588	-0.463971
H	3.855017	0.777577	-3.563739
H	2.339209	1.235206	-4.359774
H	2.934426	2.168476	-2.974400
H	0.723231	-0.498960	-4.821763
H	-0.918775	-0.250847	-5.430554
H	0.106574	1.145432	-5.058463
H	-0.779646	2.933765	-3.773267
H	0.044499	4.331374	-3.068922
H	0.980287	3.087441	-3.914544

[Ni(ZnCp*)(ZnMe)(C_2H_2)$_3$]:

Zn	2.150449	0.418056	3.757951
Zn	2.576911	2.329696	2.275060
Ni	0.953972	2.469248	4.064569
C	1.554936	-1.789859	3.696987
C	2.766910	-1.625072	2.947530
C	3.788446	-1.165711	3.849415
C	3.206260	-1.047020	5.155319
C	1.825650	-1.431778	5.061056
C	0.251008	-2.306625	3.168103
C	2.958774	-1.937060	1.494191
C	5.223646	-0.920161	3.493815
C	3.924026	-0.657555	6.412388
C	0.862638	-1.532999	6.203704
C	3.776889	2.660107	0.740115
C	2.316464	2.967933	5.568954
C	1.126292	2.514827	6.136342
C	0.250150	4.377086	3.877316
C	1.205180	4.234832	2.850232
C	-0.637110	1.627870	3.001473
C	-0.909108	1.595894	4.368433
H	0.497683	4.937345	4.780368
H	0.130627	-2.084923	2.099129
H	-0.606810	-1.866222	3.694580
H	0.172707	-3.400191	3.281103
H	3.291070	-2.977314	1.345018
H	3.715523	-1.286051	1.036411
H	2.027988	-1.810285	0.925263
H	5.683398	-0.172755	4.154175
H	5.329587	-0.557583	2.462644
H	5.823602	-1.840844	3.578643
H	4.318244	-1.539272	6.943412
H	3.263471	-0.128507	7.112933
H	4.778405	0.000540	6.204473
H	-0.174677	-1.373218	5.879164
H	0.900985	-2.527893	6.676611
H	1.081696	-0.797108	6.989538
H	3.710659	1.836983	0.014264
H	4.821988	2.721263	1.077407
H	3.535351	3.595767	0.216507
H	-0.354007	0.718739	2.473943
H	-1.549535	2.347514	4.828748
H	-0.800299	0.668510	4.929500
H	-1.047220	2.416325	2.368498
H	-0.814710	4.340807	3.641902
H	0.853625	4.152610	1.817949
H	2.164548	4.749679	2.953948
H	0.381962	3.217311	6.509795
H	1.058076	1.504734	6.538700
H	2.518143	4.035884	5.472533
H	3.200517	2.332835	5.560564

[Ni(ZnCp*)(ZnMe)(C_2H_2)$_3$]:

Zn	3.003134	2.461726	2.534514
Zn	2.537335	0.856484	4.329399
Ni	1.040563	2.698736	3.901358
C	0.407016	2.700507	1.972041
C	-0.080956	1.714439	2.586916
C	2.229981	4.370102	4.397725
C	1.091109	4.749711	4.052335
C	-0.447054	2.548645	5.316253
C	0.559774	2.040336	5.854728
C	4.071098	2.933217	0.950157
C	1.970812	-1.113362	6.914155
C	4.996654	-0.683970	5.943005
C	5.042331	-0.930863	2.756693
C	2.067776	-1.490153	1.762877
C	0.163847	-1.576861	4.342370
C	2.438865	-1.036142	5.492357
C	3.801315	-0.848233	5.053036
C	3.824170	-1.008231	3.625854

C	2.491815	-1.289166	3.186430
C	1.637882	-1.308396	4.330202
H	0.287458	5.433774	3.840150
H	3.217349	4.504843	4.804886
H	1.083573	1.617307	6.694942
H	-1.465926	2.883334	5.222576
H	-0.697021	0.835343	2.694548
H	0.463133	3.367632	1.124554
H	3.881969	3.971877	0.645659
H	5.144310	2.820807	1.154593
H	3.810929	2.274360	0.109936
H	2.557030	-0.461219	7.576986
H	2.062063	-2.137648	7.311729
H	0.914460	-0.826575	7.008415
H	5.790059	-0.100978	5.456138
H	4.739521	-0.173215	6.880722
H	5.431996	-1.659960	6.214271
H	5.517466	-1.918220	2.635835
H	4.801241	-0.562989	1.750108
H	5.799443	-0.256850	3.179423
H	1.036597	-1.151735	1.594376
H	2.710089	-0.930961	1.068973
H	2.115959	-2.550042	1.465023
H	-0.063327	-2.594768	4.697944
H	-0.373743	-0.874424	4.995822
H	-0.264975	-1.489622	3.335013

$[Ni(ZnCp^*)_2(ZnMe)_2(C_2H_4)_2]$:

Zn	-1.231231	1.437554	1.978916
Zn	1.545471	1.048979	1.986280
Zn	0.110007	0.808851	4.170247
Zn	-0.011729	0.150919	0.044009
Ni	-0.101005	-0.597736	2.283191
C	-1.964760	-1.241739	2.996182
C	-1.658518	-1.878883	1.785544
C	1.075926	-2.026847	3.224513
C	1.490530	-1.905917	1.890804
C	-0.565954	4.044646	4.971850
C	-2.644797	1.783110	5.849581
C	-0.979394	-0.732276	6.909645
C	2.130121	-0.016503	6.693865
C	-0.404654	0.533014	6.350510
C	2.381340	2.934986	5.492308
C	-0.218736	2.680970	5.485238
C	1.106260	2.179992	5.710225
C	0.553108	-2.370667	-2.049210
C	2.835505	-0.154142	-1.736862
C	1.425991	2.712976	-1.674598
C	-1.722266	2.273453	-1.957686
C	0.728561	1.390363	-1.764547
C	-2.266611	-0.868586	-2.190086
C	0.335912	-0.893761	-1.924371
C	-0.687201	1.193604	-1.881468
C	-2.524745	2.912235	1.819089
C	3.191078	2.101375	1.745285
C	-1.151891	1.665513	5.880358
C	0.993812	0.850666	6.245001
C	1.360969	0.103137	-1.791313
C	-0.932942	-0.219094	-1.979716
H	0.380566	-2.813043	3.521447
H	1.703061	-1.641423	4.026869
H	2.452634	-1.443667	1.659812
H	1.129504	-2.593216	1.126697
H	-1.212883	-2.874486	1.778302
H	-2.195575	-1.609980	0.877359
H	-1.766459	-1.726957	3.951082
H	-2.756730	-0.490558	3.030544
H	-1.514967	4.041228	4.420173
H	-0.667147	4.772774	5.792905
H	0.206870	4.429471	4.292737
H	-3.187740	2.956963	2.693699
H	-1.986819	3.868055	1.747177
H	-3.143548	2.799043	0.919177
H	3.804020	1.703337	0.925381
H	2.930860	3.142040	1.505567
H	3.795442	2.102545	2.662015
H	-3.039726	2.191759	6.793729
H	-2.980179	2.448624	5.043168
H	-3.125913	0.808065	5.693674
H	-1.963769	-0.955245	6.476367
H	-0.328961	-1.595677	6.714002
H	-1.114624	-0.669730	8.001655
H	2.395411	0.176628	7.746078
H	1.882149	-1.083846	6.616686
H	3.035329	0.157754	6.096469
H	3.219405	2.260604	5.271898
H	2.299663	3.638288	4.653065
H	2.661138	3.520915	6.382894
H	0.661095	-2.677995	-3.102113
H	1.464127	-2.691216	-1.526000
H	-0.286679	-2.942063	-1.630848
H	3.359098	0.621968	-1.163222
H	3.062164	-1.120688	-1.266811
H	3.282278	-0.171208	-2.744084
H	0.801615	3.465523	-1.174146
H	2.365305	2.639104	-1.111321
H	1.673220	3.109411	-2.672714
H	-1.878289	2.610950	-2.995224
H	-2.694324	1.930813	-1.578928
H	-1.435268	3.154694	-1.368902
H	-2.513666	-0.947737	-3.261313
H	-2.291925	-1.886936	-1.779085
H	-3.076286	-0.298724	-1.714362

$[Ni(ZnCp^*)_2(ZnMe)_2(C_2H_2)_2]$:

Zn	-2.452463	-0.423006	2.216151
Zn	2.210515	-1.023264	2.387703
Zn	0.242755	0.683110	3.415114
Zn	-0.169719	0.278407	0.752911
Ni	-0.200384	-1.336966	2.396732
C	-0.734191	-1.512276	4.202947
C	-1.962000	-1.714211	3.702827
C	1.344178	-2.546793	1.359131
C	0.194064	-2.206286	0.760236
C	-1.776582	3.364639	3.280625
C	-2.703909	1.196035	5.381611
C	-0.084397	0.192125	7.005323
C	2.438800	1.668324	5.801806
C	-0.119775	1.148606	5.850532
C	1.415199	3.717282	3.544260
C	-0.862212	2.545627	4.144170
C	0.584012	2.667748	4.222730
C	-0.121574	-1.319987	-2.461712
C	2.733459	-0.589940	-1.113775
C	2.491404	2.276645	0.192268
C	-0.502465	3.356414	-0.302412
C	1.362897	1.508496	-0.430599
C	-2.114867	1.069599	-1.885881
C	0.210005	-0.100152	-1.654429
C	-0.000102	1.975301	-0.605071
C	-3.731386	0.779553	1.328836
C	3.804819	0.006451	2.905501
C	-1.283278	1.614179	5.151146
C	1.035795	1.781180	5.280136
C	1.483073	0.235887	-1.082714
C	-0.714236	0.959055	-1.357148
H	-2.680133	-2.464929	4.089434
H	-0.259755	-1.811164	5.151558
H	1.831925	-3.537548	1.263998
H	-0.375372	-2.659563	-0.067277
H	-2.697430	2.808890	3.018322
H	-2.093083	4.298186	3.797316
H	-1.293726	3.664652	2.332068
H	-4.566937	1.039488	2.012089
H	-3.251497	1.721090	0.996076
H	-4.164680	0.286167	0.434110
H	4.642069	-0.185854	2.202267
H	3.608813	1.096717	2.920092
H	4.138360	-0.291378	3.921284
H	-3.338454	2.045773	5.713362
H	-3.166935	0.788047	4.455062
H	-2.777602	0.398607	6.144989
H	-1.019162	-0.396428	7.084345
H	0.757966	-0.526363	6.921462
H	0.051094	0.724928	7.972586
H	2.590449	2.312931	6.696216
H	2.683853	0.630795	6.106934
H	3.187960	1.972038	5.046377
H	2.452966	3.375978	3.360751
H	0.981938	4.016697	2.569667
H	1.478143	4.637687	4.166325
H	-0.145648	-1.094601	-3.550918
H	0.619543	-2.129014	-2.311372
H	-1.120686	-1.728644	-2.202224
H	3.117292	-0.794046	-0.088989
H	2.561691	-1.575953	-1.585259
H	3.551046	-0.083474	-1.670372
H	2.139848	2.956771	0.990383
H	3.243433	1.601951	0.644653
H	3.021787	2.901188	-0.560811
H	-0.354318	4.033465	-1.172865
H	-1.583878	3.365901	-0.062466
H	0.036472	3.809566	0.552770
H	-2.121698	1.437649	-2.936097
H	-2.635787	0.090852	-1.883535
H	-2.730080	1.768653	-1.288330

$[Ni(ZnCp^*)_3(ZnMe)_3(C_2H_4)]$:

Zn	-1.480808	-2.524569	1.358427
Zn	-1.520155	-1.591592	4.105942
Zn	-1.724233	0.044549	1.912448
Zn	2.006216	0.124624	2.049990
Zn	0.026736	0.808878	3.699429
Zn	0.310044	-0.878786	0.228779
Ni	0.150889	-1.253403	2.523993
C	-0.380569	-5.627924	0.736655
C	-2.193634	-5.267283	3.340165
C	-2.400687	-4.579549	2.026455
C	-1.726796	-3.988309	-1.633149
C	-4.597050	-3.274902	2.598607
C	-3.479022	-3.695310	1.695367
C	-4.307853	-2.473051	-0.451793
C	-3.340469	-3.318226	0.318978
C	-2.174390	-3.977650	-0.205087
C	-1.586289	-4.746485	0.859243
C	-2.777326	-2.036805	5.557161
C	0.001799	0.308338	7.081664
C	-1.624795	3.770989	3.608192
C	1.575068	3.799141	3.625481
C	2.239973	2.652591	-0.044045
C	0.859258	-1.450560	-2.824176
C	-0.854327	2.694606	-0.260489
C	-2.606559	1.633821	5.730117
C	2.566167	1.622113	5.740233
C	3.338929	-0.037219	-1.464338
C	-1.790393	0.156997	-2.020760

C	1.752740	-2.496272	2.825806
C	-3.420293	0.971379	1.523537
C	3.874991	0.732231	2.293774
C	-1.177675	1.901926	5.371221
C	-0.737699	2.853577	4.391157
C	0.697959	2.856183	4.387598
C	1.143254	1.891897	5.359612
C	-0.017154	1.310443	5.969005
C	0.007326	1.590432	-0.786511
C	-0.413774	0.432423	-1.495005
C	0.771691	-0.366747	-1.785978
C	1.909739	0.360259	-1.260084
C	1.429905	1.551511	-0.655887
C	0.795576	-2.690782	3.855883
H	0.201733	-3.606877	3.852333
H	1.021642	-2.305951	4.852226
H	1.819143	-3.217266	2.011999
H	2.704254	-2.018386	3.073545
H	-0.652617	-6.648183	0.420524
H	0.155298	-5.718497	1.691196
H	0.330274	-5.238848	-0.004907
H	-2.738365	-6.224328	3.382246
H	-1.133822	-5.496553	3.516743
H	-2.546730	-4.657755	4.181418
H	-2.132885	-4.860066	-2.171685
H	-0.633092	-4.034950	-1.720340
H	-2.065740	-3.093164	-2.170515
H	-5.490029	-3.903821	2.451725
H	-4.314880	-3.348409	3.655538
H	-4.899848	-2.235532	2.410165
H	-5.153093	-3.071548	-0.828570
H	-3.832561	-1.998243	-1.319191
H	-4.728384	-1.671734	0.170261
H	-2.953250	-3.119294	5.622572
H	-3.743785	-1.544984	5.381946
H	-2.397396	-1.705925	6.533310
H	-2.589442	3.301035	3.377700
H	-1.837588	4.696002	4.168493
H	-1.166844	4.067814	2.655479
H	-4.167325	0.670290	2.272793
H	-3.315063	2.062549	1.563297
H	-3.807372	0.694565	0.533507
H	4.508099	0.423771	1.450241
H	3.941265	1.823887	2.387582
H	4.292412	0.286873	3.208316
H	-2.993394	2.393251	6.428582
H	-3.255362	1.649398	4.843372
H	-2.728363	0.655407	6.209088
H	-0.929492	-0.269006	7.123579
H	0.830034	-0.405652	6.972007
H	0.127143	0.797657	8.060993
H	2.887388	2.267103	6.574278
H	2.708846	0.581923	6.062967
H	3.249923	1.803300	4.901815
H	2.532346	3.336723	3.352023
H	1.093776	4.142411	2.700418
H	1.804866	4.696702	4.222515
H	1.072134	-1.025017	-3.819140
H	1.659569	-2.169534	-2.602250
H	-0.077291	-2.014763	-2.905411
H	4.002746	0.452290	-0.741394
H	3.480527	-1.121861	-1.361145
H	3.689853	0.238951	-2.472566
H	1.893240	2.910924	0.967966
H	3.301413	2.391446	0.029792
H	2.163431	3.573485	-0.644756
H	-0.617156	3.653444	-0.748745
H	-1.919833	2.494623	-0.419591
H	-0.707222	2.845322	0.821099
H	-1.934691	0.603520	-3.018033
H	-1.976758	-0.920194	-2.118841
H	-2.567493	0.563137	-1.361043

$[Ni(ZnCp^*)_3(ZnMe)_3(C_2H_2)]$:

Zn	-1.473038	-2.509591	1.284692
Zn	-1.530252	-1.571563	4.127962
Zn	-1.769412	0.010051	1.922856
Zn	2.084403	-0.013844	2.160901
Zn	0.024099	0.890506	3.583355
Zn	0.296156	-0.872813	0.246758
Ni	0.137063	-1.261773	2.545242
C	-0.271707	-5.549574	0.719405
C	-2.033766	-5.170063	3.332867
C	-2.315306	-4.548535	2.000311
C	-1.729857	-4.036912	-1.688504
C	-4.554896	-3.310233	2.567734
C	-3.432871	-3.715892	1.662920
C	-4.338329	-2.581443	-0.500603
C	-3.330820	-3.374757	0.273607
C	-2.152558	-4.007664	-0.253253
C	-1.516713	-4.722141	0.822368
C	-2.854328	-1.965408	5.529982
C	-0.063837	0.241322	6.956545
C	-1.450521	3.912204	3.586310
C	1.756526	3.788667	3.699165
C	2.084908	2.595821	0.154326
C	0.798091	-1.408125	-2.827742
C	-0.989346	2.653703	-0.178778
C	-2.587480	1.753806	5.600084
C	2.572570	1.457644	5.725857
C	3.247757	0.004429	-1.409075
C	-1.879596	0.136476	-2.000939
C	1.691891	-2.425962	2.974686

C	-3.497487	0.900112	1.589669
C	3.969366	0.549503	2.321619
C	-1.136808	1.961260	5.289977
C	-0.625892	2.924693	4.353217
C	0.809110	2.855940	4.386023
C	1.178459	1.832623	5.328100
C	-0.021890	1.294475	5.892390
C	-0.110044	1.573988	-0.726842
C	-0.508013	0.431097	-1.474974
C	0.686101	-0.345582	-1.771621
C	1.810805	0.372676	-1.198907
C	1.308874	1.543232	-0.570466
C	0.759444	-2.657013	3.822567
H	0.522469	-3.294923	4.668517
H	2.671795	-2.761529	2.656211
H	0.316095	-5.507689	1.646399
H	0.376077	-5.201006	-0.095869
H	-0.501984	-6.609482	0.523918
H	-2.428649	-6.197089	3.391471
H	-0.954033	-5.228207	3.528140
H	-2.490342	-4.599820	4.151444
H	-2.132499	-4.923496	-2.204934
H	-0.637297	-4.069870	-1.793608
H	-2.090784	-3.155793	-2.235004
H	-5.437671	-3.954092	2.424596
H	-4.269629	-3.375760	3.624030
H	-4.875327	-2.276388	2.377386
H	-5.173104	-3.214650	-0.842662
H	-3.894874	-2.118589	-1.391167
H	-4.769960	-1.774801	0.107134
H	-3.043393	-3.044463	5.612386
H	-3.805619	-1.469423	5.294794
H	-2.514591	-1.611340	6.512127
H	-2.400635	3.474434	3.251857
H	-1.696807	4.792799	4.201756
H	-0.923749	4.276715	2.694930
H	-4.236391	0.514228	2.307142
H	-3.432774	1.988328	1.715399
H	-3.867743	0.687721	0.577665
H	4.567567	0.192158	1.472141
H	4.062125	1.642123	2.371191
H	4.397719	0.125822	3.240737
H	-2.958852	2.512320	6.307757
H	-3.206640	1.823967	4.695040
H	-2.771510	0.769245	6.046067
H	-1.083583	-0.124067	7.121472
H	0.563354	-0.626024	6.701210
H	0.304508	0.631529	7.918421
H	2.893221	2.003328	6.628425
H	2.652890	0.385099	5.949348
H	3.294468	1.684036	4.931660
H	2.685397	3.283931	3.402030
H	1.313092	4.229548	2.797440
H	2.037213	4.622210	4.363488
H	1.010258	-0.961149	-3.813437
H	1.608484	-2.117773	-2.613016
H	-0.129023	-1.985276	-2.925340
H	3.901196	0.487452	-0.672714
H	3.409766	-1.079508	-1.332329
H	3.593790	0.311952	-2.409731
H	1.759581	2.692437	1.203075
H	3.160328	2.385900	0.162960
H	1.939149	3.584819	-0.308351
H	-0.756391	3.627918	-0.637844
H	-2.051042	2.448382	-0.355287
H	-0.854030	2.776261	0.908020
H	-2.037961	0.592546	-2.991657
H	-2.043028	-0.943504	-2.110749
H	-2.662370	0.517427	-1.332892

$[Ni(AlCp^*)(C_2H_4)_3]$:

C	-4.750181	-0.340899	1.078494
C	-4.638115	0.996352	0.576189
C	-4.377731	0.920464	-0.831728
C	-4.322045	-0.462803	-1.197069
C	-4.549211	-1.242098	-0.016243
Al	-2.631292	-0.042546	0.263693
Ni	-0.389370	-0.136409	0.078867
C	-4.222411	2.089415	-1.756811
C	-4.080724	-1.008988	-2.571826
C	-4.806603	2.256115	1.370974
H	-4.518952	2.114769	2.420899
H	-4.196758	3.074740	0.966869
H	-5.854788	2.593690	1.361283
H	-3.752730	2.945055	-1.253998
H	-3.604614	1.838993	-2.628046
H	-5.200245	2.428371	-2.132909
H	-3.475908	-1.925161	-2.545037
H	-5.028989	-1.256389	-3.073658
H	-3.555176	-0.284560	-3.206547
C	-0.636522	-2.076654	-0.619477
C	0.515773	-1.975876	0.170929
H	-0.569534	-2.041118	-1.708766
H	-1.502961	-2.617384	-0.238775
H	1.496638	-1.865382	-0.291026
H	0.520525	-2.374679	1.184863
C	0.867246	0.453427	1.596503
C	-0.012449	1.497583	1.300156
H	1.879102	0.449652	1.190817
H	0.718160	-0.158856	2.485546
H	0.296374	2.321440	0.654027
H	-0.830813	1.732194	1.978486
C	0.635587	0.594353	-1.600521

C	-0.703986	0.930475	-1.785505
H	1.069239	-0.260944	-2.120565
H	1.352498	1.334229	-1.242350
H	-1.323829	0.352742	-2.471599
H	-1.052674	1.944021	-1.590239
C	-5.045969	-0.730914	2.494672
H	-4.582759	-1.691747	2.754945
H	-6.129980	-0.834354	2.658938
H	-4.677301	0.018473	3.207151
C	-4.601918	-2.738559	0.052657
H	-3.994868	-3.200862	-0.736495
H	-5.632816	-3.105073	-0.072440
H	-4.237317	-3.115068	1.017603

$[Ni(AlCp^*)(C_2H_2)_3]$:

C	-4.209822	-0.417060	0.852416
C	-4.174727	0.915054	0.297595
C	-4.366028	0.810962	-1.112765
C	-4.486791	-0.583578	-1.443505
C	-4.421698	-1.335927	-0.218694
Al	-2.474486	-0.266380	-0.549256
Ni	-0.458633	0.271108	0.798489
C	-4.382252	1.945960	-2.088176
C	-4.740015	-1.145271	-2.810709
C	-3.979659	2.177099	1.079640
H	-3.322862	2.012214	1.943515
H	-3.522027	2.963413	0.465806
H	-4.938583	2.565322	1.456458
H	-3.807970	2.803464	-1.714998
H	-3.950154	1.655666	-3.054980
H	-5.409089	2.295245	-2.278343
H	-4.333608	-2.159767	-2.914684
H	-5.819228	-1.202614	-3.022172
H	-4.287327	-0.524116	-3.594626
C	-1.086480	-1.605607	-0.094164
C	0.126579	-1.160028	-0.610215
C	-0.529909	0.375343	2.660093
C	-0.502875	1.556585	2.150976
C	0.158880	0.191854	-1.198593
C	-1.025957	0.921624	-1.194675
C	-4.052462	-0.758708	2.301890
H	-3.642649	-1.768168	2.434431
H	-5.018509	-0.720544	2.828735
H	-3.370552	-0.059527	2.803035
C	-4.507451	-2.825429	-0.099721
H	-4.100595	-3.327059	-0.987610
H	-5.550767	-3.157817	0.016827
H	-3.947511	-3.190985	0.770540
H	-0.540105	2.628734	2.305798
H	-0.605862	-0.246795	3.544414
H	-0.981947	1.962497	-1.519503
H	1.119364	0.592656	-1.536240
H	-1.090224	-2.553004	0.447400
H	1.064160	-1.718330	-0.530303

$[Ni(AlCp^*)_2(C_2H_4)_2]$:

Al	-2.135926	-0.255143	0.186728
Ni	-0.096332	0.466066	-0.256512
C	1.206908	1.282771	1.122370
C	0.126583	2.156259	0.879550
C	0.664956	0.951593	-2.095821
C	-0.735574	1.116702	-2.110088
H	1.122921	0.122527	-2.632813
H	1.318943	1.810875	-1.932665
H	-1.350786	0.418541	-2.678330
H	-1.171011	2.109287	-1.988642
C	-4.235754	0.387581	-0.453123
C	-4.239710	0.198209	0.966156
C	-4.517120	1.255206	1.991534
H	-4.012730	1.038799	2.942412
H	-5.595368	1.332762	2.202399
H	-4.178140	2.243467	1.653752
C	-3.947304	-1.179645	1.232228
C	-3.756302	-1.838853	-0.025255
C	-3.933802	-0.869829	-1.066068
C	-3.838896	-1.151784	-2.534862
H	-3.012677	-1.839129	-2.763714
H	-4.764238	-1.615878	-2.910609
H	-3.674972	-0.233695	-3.112291
C	-4.481140	1.684995	-1.160949
H	-4.066731	2.533715	-0.600499
H	-5.558509	1.871171	-1.291900
H	-4.020563	1.693659	-2.156543
Al	0.707706	-1.542946	0.181865
C	1.057469	-3.803047	0.182465
C	0.764731	-3.384623	1.520805
C	-0.389318	-3.825938	2.366873
H	-0.811819	-2.990797	2.943019
H	-0.082664	-4.599559	3.088152
H	-1.195356	-4.250693	1.755766
C	1.799465	-2.487200	1.941926
C	2.733238	-2.351933	0.866003
C	2.273244	-3.160409	-0.222859
C	2.955281	-3.318076	-1.547878
H	3.486988	-2.402609	-1.839175
H	3.695866	-4.132867	-1.520585
H	2.239169	-3.553780	-2.346011

C	0.259763	-4.768593	-0.640069
H	-0.793071	-4.788465	-0.331467
H	0.651019	-5.793326	-0.541619
H	0.286271	-4.510820	-1.707501
C	-3.890947	-1.818799	2.586260
H	-3.488338	-1.132078	3.343099
H	-3.258316	-2.715301	2.583516
H	-4.893637	-2.125111	2.923403
C	-3.464828	-3.291833	-0.239576
H	-3.036149	-3.751485	0.659715
H	-2.753856	-3.444472	-1.063394
H	-4.380428	-3.850757	-0.488805
C	1.881433	-1.835494	3.288914
H	0.895289	-1.498315	3.637287
H	2.544181	-0.961610	3.274919
H	2.274041	-2.534043	4.044395
C	3.964405	-1.498228	0.859973
H	3.885341	-0.672207	1.577642
H	4.142694	-1.056705	-0.129627
H	4.858209	-2.084045	1.125360
H	-0.640996	2.300045	1.638203
H	0.234195	2.981301	0.172178
H	1.274726	0.769351	2.081794
H	2.164819	1.446165	0.627140

$[Ni(AlCp^*)_2(C_2H_2)_2]$:

Ni	0.019404	0.841300	0.106412
Al	0.332515	-1.770185	-0.038551
Al	-1.913055	-0.651131	-0.105387
C	3.408126	-0.994069	0.779626
C	1.324663	-1.611481	3.134365
C	-3.880647	-3.335779	-0.297483
C	-3.689782	-1.842041	2.521522
C	0.565635	-5.075008	-0.619812
C	2.933939	-3.115014	-1.538732
C	2.170215	-3.042372	-0.252376
C	2.379433	-2.082509	0.787615
C	1.454815	-2.375699	1.853070
C	-0.425404	-4.132053	2.251999
C	0.691298	-3.518141	1.469861
C	1.110867	-3.918153	0.161406
C	-3.825159	1.768675	-1.158219
C	-4.001863	-1.115926	-2.586648
C	-3.874193	-0.851191	-1.116263
C	-3.857015	-1.855689	-0.076753
C	-3.786621	-1.191043	1.177707
C	-3.692936	1.303285	1.966955
C	-3.743975	0.223662	0.929639
C	-3.841360	0.433364	-0.481767
C	-0.673693	0.340793	-1.611425
C	0.405626	-0.504870	-1.637787
C	-0.056548	1.768623	1.748850
C	1.137890	1.782045	1.304468
H	-0.949650	1.025784	-2.422720
H	2.179548	2.066648	1.375416
H	-0.781756	2.012228	2.514127
H	1.148545	-0.457159	-2.447356
H	4.412000	-1.393197	0.993291
H	3.454559	-0.484801	-0.193194
H	3.183480	-0.234217	1.537057
H	2.023333	-1.986036	3.898672
H	1.525902	-0.542704	2.986117
H	0.310365	-1.694901	3.546576
H	-4.911642	-3.718566	-0.354863
H	-3.373955	-3.611519	-1.232203
H	-3.375745	-3.868598	0.519073
H	-4.676251	-1.924649	3.003875
H	-3.275381	-2.855656	2.446727
H	-3.041876	-1.270398	3.200812
H	0.699158	-4.932203	-1.700183
H	1.071304	-6.015260	-0.348913
H	-0.507880	-5.216624	-0.434433
H	2.321743	-3.523032	-2.353890
H	3.821416	-3.760080	-1.440722
H	3.284174	-2.122985	-1.852457
H	-1.208466	-4.526862	1.589066
H	-0.075191	-4.967478	2.878328
H	-0.897802	-3.397570	2.917743
H	-3.678485	1.667760	-2.240149
H	-4.771447	2.308055	-1.000145
H	-3.012632	2.402941	-0.773700
H	-3.549771	-0.312766	-3.182062
H	-5.058393	-1.197817	-2.886054
H	-3.506826	-2.053259	-2.872433
H	-3.185439	2.198942	1.586115
H	-4.705921	1.603769	2.277943
H	-3.160764	0.972397	2.868701

$[Ni(AlCp^*)_3(C_2H_4)]$:

Ni	0.047786	0.476237	-0.430965
C	0.595970	0.162472	-2.358652
C	-0.515160	1.032333	-2.300725
H	0.460744	-0.864996	-2.697638
H	1.601074	0.561114	-2.494177
H	-1.500678	0.668447	-2.594631
H	-0.378161	2.109552	-2.397568
Al	0.378233	-1.556093	0.381013
C	0.876810	-3.621358	-0.514288
C	0.212227	-3.820406	0.738076
C	-1.067347	-4.572516	0.935111
H	-1.566149	-4.287863	1.869991
H	-0.885180	-5.658020	0.979452

H	-1.774799	-4.397734	0.112408
C	1.027336	-3.246149	1.770096
C	2.198932	-2.705109	1.148945
C	2.101745	-2.930985	-0.259109
C	3.105006	-2.459180	-1.265961
H	3.365597	-1.403840	-1.099672
H	4.034716	-3.046416	-1.209392
H	2.720676	-2.544598	-2.289343
C	0.362002	-4.064208	-1.849906
H	-0.729833	-3.961069	-1.916745
H	0.603122	-5.121435	-2.042479
H	0.798200	-3.473991	-2.665627
C	0.726098	-3.261986	3.238490
H	-0.354214	-3.207309	3.429405
H	1.193943	-2.413968	3.755337
H	1.096256	-4.183474	3.714825
C	3.332944	-1.991651	1.815972
H	3.156930	-1.877385	2.892023
H	3.477544	-0.985862	1.391031
H	4.277761	-2.541633	1.690434
Al	1.322456	1.636357	0.983847
C	1.247203	3.721163	1.968654
C	2.607639	3.464602	1.609947
C	3.434380	4.250095	0.637932
H	4.167157	3.613062	0.124633
H	3.995289	5.051175	1.145100
H	2.812056	4.722827	-0.133100
C	3.058498	2.330813	2.360923
C	1.971793	1.883106	3.178759
C	0.855657	2.743943	2.934703
C	-0.491373	2.637465	3.574254
H	-0.705558	1.608372	3.889958
H	-0.571804	3.281381	4.464723
H	-1.284509	2.938240	2.875667
C	0.357287	4.790248	1.413210
H	0.741907	5.180127	0.462395
H	0.265034	5.640190	2.107355
H	-0.655637	4.405520	1.224116
Al	-1.908242	0.749348	0.545104
C	-3.988337	1.261817	-0.259923
C	-3.863272	1.836874	1.046028
C	-3.948519	3.298646	1.363057
H	-3.471861	3.534508	2.323228
H	-4.995747	3.633555	1.427933
H	-3.459374	3.909014	0.591385
C	-3.686719	0.767674	1.985657
C	-3.616602	0.891102	3.476848
H	-3.299536	1.893015	3.789064
H	-2.913921	0.169247	3.915377
H	-4.602139	0.701980	3.930631
C	-3.698672	-0.463984	1.254416
C	-3.540488	-1.837397	1.826364
H	-2.988897	-1.818662	2.775614
H	-2.988756	-2.489721	1.137097
H	-4.516490	-2.309739	2.020047
C	-3.890040	-0.159584	-0.129710
C	-3.902667	-1.171370	-1.234494
H	-3.044735	-1.856271	-1.153112
H	-4.819546	-1.779567	-1.213288
H	-3.845174	-0.692368	-2.219296
C	-4.181292	2.034866	-1.528819
H	-3.583856	2.956528	-1.534842
H	-5.235159	2.324717	-1.662647
H	-3.885773	1.449345	-2.407902
C	4.443476	1.760484	2.320916
H	5.140670	2.366291	2.921061
H	4.841267	1.726700	1.296918
H	4.472529	0.738600	2.718718
C	1.984210	0.741917	4.149807
H	2.851424	0.090313	3.990722
H	1.081927	0.119655	4.056189
H	2.027987	1.100725	5.189836

$[Ni(AlCp^*)_3(C_2H_2)]$:

Ni	0.252040	0.171399	-0.526441
Al	-1.743980	0.931298	0.143267
Al	1.334336	1.641106	0.739440
Al	0.436069	-1.447305	1.064932
C	2.672203	0.760911	3.664343
C	4.506573	2.351621	1.542632
C	-3.976237	3.306092	-0.699932
C	-3.908333	0.594877	-2.364735
C	-3.777230	0.707837	-0.876064
C	-3.478681	-1.825692	-0.264177
C	-3.613696	-0.369051	0.051191
C	-3.308115	-0.613919	2.616306
C	-3.516705	0.185716	1.366785
C	-3.721122	2.590521	2.384268
C	-3.634661	1.609953	1.255666
C	-3.786642	1.932146	-0.133456
C	-0.230033	4.439680	1.538304
C	-0.206369	2.014487	3.615301
C	0.953071	2.493940	2.797035
C	2.257833	1.907702	2.797822
C	3.064005	2.615781	1.850639
C	2.712385	4.650111	0.250103
C	2.253917	3.651874	1.270361
C	0.953100	3.581718	1.866891
C	3.543158	-2.364055	2.018262
C	1.093159	-2.985535	4.040976
C	-0.397429	-4.134634	-0.772593
C	2.591235	-3.071537	-0.901513
C	1.755872	-3.193575	0.334628

C	2.179512	-2.870488	1.660547
C	1.090524	-3.133796	2.549654
C	-1.316684	-4.102082	2.319063
C	-0.002671	-3.637028	1.769495
C	0.411650	-3.676056	0.402006
C	-0.183217	-0.616435	-2.246409
C	1.044194	-0.272560	-2.244161
H	-1.012198	-1.052938	-2.787421
H	1.989588	-0.207480	-2.764734
H	2.789897	1.079241	4.711966
H	1.921172	-0.043060	3.645590
H	3.626459	0.331891	3.338369
H	4.768723	1.299171	1.713071
H	4.746124	2.585571	0.496887
H	5.168924	2.963019	2.175342
H	-3.569183	3.382264	-1.716890
H	-5.043717	3.573331	-0.752851
H	-3.478691	4.068504	-0.085609
H	-3.334513	1.375314	-2.882561
H	-4.958471	0.692096	-2.680898
H	-3.542892	-0.373471	-2.727447
H	-4.297828	-2.410376	0.180974
H	-3.486191	-2.008335	-1.345084
H	-2.529687	-2.222399	0.128536
H	-4.193820	-1.221464	2.857584
H	-2.455192	-1.302475	2.507310
H	-3.101636	0.031041	3.479317
H	-3.177497	3.520563	2.168644
H	-4.769511	2.866722	2.578300
H	-3.316805	2.174680	3.314944
H	-1.071325	3.831794	1.163803
H	-0.582323	4.992839	2.421291
H	0.011658	5.173273	0.760138
H	-1.118210	2.565546	3.361640
H	-0.021976	2.147252	4.692320
H	-0.404458	0.943782	3.444546
H	1.884237	4.991746	-0.383885
H	3.151739	5.538334	0.730563
H	3.477627	4.225068	-0.412661
H	4.309947	-3.133260	1.839004
H	3.818641	-1.483504	1.417478
H	3.603656	-2.079391	3.075187
H	1.274807	-3.951467	4.538687
H	1.874672	-2.292720	4.378394
H	0.131979	-2.603867	4.413488
H	-0.299378	-3.439322	-1.618077
H	-0.070226	-5.127558	-1.118441
H	-1.463339	-4.209474	-0.524549
H	1.966363	-2.931602	-1.791786
H	3.208028	-3.971610	-1.056165
H	3.268448	-2.209137	-0.841187
H	-2.121101	-4.025879	1.576116
H	-1.264722	-5.155665	2.637468
H	-1.620807	-3.514262	3.196071

[Ni(GaCp*)(C_2H_4)$_3$]:

C	-4.821981	-0.341036	1.126116
C	-4.743775	0.994297	0.606858
C	-4.418991	0.907733	-0.787454
C	-4.292158	-0.476311	-1.126702
C	-4.536908	-1.247900	0.054574
Ga	-2.566480	0.057195	0.461998
Ni	-0.254879	-0.096177	-0.013779
C	-4.290450	2.066110	-1.729285
C	-3.991577	-1.030201	-2.485798
C	-5.036993	2.253017	1.365452
H	-4.787210	2.154223	2.430256
H	-4.471922	3.107438	0.969623
H	-6.105694	2.515075	1.305353
H	-3.897670	2.958887	-1.224314
H	-3.617680	1.837738	-2.565810
H	-5.266274	2.340780	-2.160991
H	-3.370857	-1.934780	-2.430864
H	-4.915077	-1.301740	-3.021705
H	-3.458673	-0.301844	-3.110758
C	-0.559494	-1.998462	-0.806245
C	0.463094	-2.029245	0.140269
H	-0.340914	-1.942939	-1.873325
H	-1.541187	-2.403756	-0.561474
H	1.508125	-1.988366	-0.169008
H	0.285775	-2.437063	1.134788
C	0.939588	0.326626	1.622738
C	0.327510	1.498815	1.185432
H	1.969198	0.101931	1.342748
H	0.567346	-0.204032	2.498691
H	0.867097	2.213642	0.563034
H	-0.528988	1.907864	1.719563
C	0.663759	0.633509	-1.712703
C	-0.670810	1.023317	-1.793593
H	1.029181	-0.223909	-2.279914
H	1.434178	1.336800	-1.394560
H	-1.368384	0.471617	-2.422584
H	-0.971367	2.037408	-1.533263
C	-5.198771	-0.721991	2.525043
H	-4.730102	-1.667603	2.828938
H	-6.288540	-0.853441	2.622999
H	-4.898644	0.045517	3.250886
C	-4.555337	-2.744086	0.139751
H	-3.896441	-3.201887	-0.610256
H	-5.567759	-3.142524	-0.035075
H	-4.233260	-3.101014	1.127280

[Ni(GaCp*)(C_2H_2)$_3$]:

Ga	-2.556717	0.203803	1.075613
Ni	0.214078	-0.062112	-0.518286
C	-4.441974	-2.754230	0.444819
C	-5.759709	-0.697689	2.509727
C	-0.366801	1.589808	-1.466080
C	-0.306597	0.660023	-2.303390
C	1.064060	1.236775	0.734544
C	1.023264	0.117493	1.294761
C	0.194205	-2.008839	-0.136338
C	-0.132847	-1.840292	-1.334561
C	-5.544651	2.228830	1.256815
C	-3.458291	-1.097077	-2.094233
C	-4.103191	1.980465	-1.587661
C	-4.493437	-1.263010	0.296552
C	-4.033190	-0.518645	-0.839137
C	-4.334543	0.864825	-0.613459
C	-4.991564	0.971361	0.656351
C	-5.091320	-0.341276	1.216000
H	-0.416969	0.216655	-3.277738
H	1.206833	-0.576502	2.096791
H	-0.524089	2.602728	-1.137454
H	0.410644	-2.595271	0.740091
H	-0.443290	-2.157911	-2.314634
H	1.278362	2.289167	0.661541
H	-4.403005	-3.056489	1.500262
H	-5.330212	-3.236391	0.003606
H	-3.560890	-3.180971	-0.053914
H	-5.683582	0.115415	3.244697
H	-6.833545	-0.904289	2.367497
H	-5.316961	-1.595318	2.962704
H	-2.749740	-0.403686	-2.566753
H	-4.245493	-1.316565	-2.834712
H	-2.926328	-2.037102	-1.896400
H	-4.957993	2.102045	-2.273812
H	-3.212927	1.798625	-2.204465
H	-3.962755	2.943506	-1.077299
H	-6.591476	2.395906	0.952977
H	-4.974156	3.114136	0.944185
H	-5.530012	2.196692	2.354921

[Ni(GaCp*)$_2$(C_2H_4)$_2$]:

Ga	-2.275809	0.536745	0.040331
Ni	0.085831	0.627666	-0.177548
C	0.720815	1.459418	1.621597
C	0.966047	2.306271	0.538210
C	1.143557	0.676608	-1.899106
C	-0.119888	0.142663	-2.176112
H	2.007297	0.023687	-1.761208
H	1.379642	1.705214	-2.173319
H	-0.260823	-0.931915	-2.288465
H	-0.873445	0.758175	-2.668303
C	-4.602632	0.422760	-0.458211
C	-4.408804	-0.229220	0.807051
C	-4.991390	0.208997	2.116221
H	-4.377819	-0.120796	2.965172
H	-6.001697	-0.205775	2.263570
H	-5.078504	1.302192	2.176552
C	-3.628747	-1.406173	0.577313
C	-3.343811	-1.485695	-0.822021
C	-3.940758	-0.356899	-1.463152
C	-3.933249	-0.061051	-2.932463
H	-3.056364	-0.495470	-3.429597
H	-4.827534	-0.470181	-3.429515
H	-3.921271	1.019723	-3.129005
C	-5.433536	1.645952	-0.699209
H	-5.432698	2.316494	0.170572
H	-6.483694	1.381904	-0.904996
H	-5.069695	2.220795	-1.561459
Ga	0.334976	-1.514361	0.741381
C	0.842542	-3.863229	0.795384
C	1.005591	-3.334774	2.119676
C	0.236389	-3.753171	3.335216
H	0.161827	-2.939255	4.068808
H	0.721048	-4.603771	3.841255
H	-0.785235	-4.066337	3.082095
C	2.095473	-2.404093	2.090749
C	2.600659	-2.355466	0.753231
C	1.824652	-3.251080	-0.048267
C	2.017253	-3.520922	-1.510064
H	2.396958	-2.637128	-2.039933
H	2.738025	-4.336789	-1.679452
H	1.076224	-3.814458	-1.994192
C	-0.129320	-4.929408	0.392375
H	-1.067369	-4.865114	0.960212
H	0.287567	-5.934310	0.567813
H	-0.383777	-4.866612	-0.673672
C	-3.192613	-2.409018	1.598922
H	-3.269897	-2.012165	2.619211
H	-2.144115	-2.709430	1.441534
H	-3.802517	-3.325583	1.553151
C	-2.554153	-2.578414	-1.471088
H	-1.587746	-2.733050	-0.962846
H	-2.342368	-2.354792	-2.523848
H	-3.091586	-3.538929	-1.437907
C	2.649544	-1.661643	3.268525
H	1.866502	-1.400938	3.993312
H	3.143760	-0.729702	2.963151
H	3.400637	-2.264188	3.804423
C	3.744886	-1.510832	0.282949
H	3.741262	-0.519208	0.756320
H	3.710478	-1.355812	-0.803180
H	4.714611	-1.979950	0.513358

H	0.281528	3.122762	0.301781
H	1.974621	2.409516	0.137196
H	-0.143279	1.608474	2.267744
H	1.541244	0.899783	2.071845

$[Ni(GaCp^*)_2(C_2H_2)_2]$:

Ga	0.148443	-1.550296	1.122315
Ga	-2.313291	0.392538	0.062593
Ni	-0.077635	0.871723	-0.042174
C	3.368430	-1.210874	0.064874
C	2.925760	-1.782458	3.158094
C	-2.595612	-2.737377	-1.297430
C	-3.484435	-2.352378	1.698690
C	-0.020285	-5.085209	0.501321
C	1.515877	-3.214401	-1.596419
C	1.582701	-3.111682	-0.102451
C	2.402067	-2.200055	0.638522
C	2.213367	-2.471354	2.033469
C	0.834193	-4.194145	3.427899
C	1.294621	-3.561206	2.150434
C	0.903508	-3.953746	0.835912
C	-5.238433	1.701224	-1.005065
C	-3.712894	-0.236710	-3.007697
C	-3.854619	-0.450035	-1.531339
C	-3.376612	-1.569754	-0.780411
C	-3.747138	-1.381241	0.590220
C	-5.107971	0.413400	1.923572
C	-4.453306	-0.133815	0.692099
C	-4.520916	0.441719	-0.627541
C	0.002653	0.173090	-1.873257
C	1.080999	0.774520	-1.605152
C	1.202807	1.868522	1.048882
C	0.084702	1.893269	1.631795
H	2.243382	2.126780	0.935055
H	-0.557974	2.172864	2.450794
H	2.069546	1.135654	-1.838733
H	-0.613927	-0.392816	-2.553553
H	4.391951	-1.619386	0.037362
H	3.095175	-0.937180	-0.961445
H	3.402320	-0.284975	0.655664
H	3.892959	-2.263265	3.379335
H	3.133319	-0.730235	2.920513
H	2.335968	-1.800847	4.084603
H	-3.205691	-3.653213	-1.318372
H	-2.229203	-2.563017	-2.316651
H	-1.720723	-2.942069	-0.660849
H	-4.234517	-3.159172	1.703386
H	-2.493601	-2.818279	1.596507
H	-3.516148	-1.866480	2.682128
H	-0.460179	-4.969143	-0.498158
H	0.506434	-6.053651	0.509486
H	-0.848227	-5.165962	1.220430
H	0.545833	-3.606621	-1.932140
H	2.291732	-3.889999	-1.992281
H	1.655479	-2.234891	-2.072232
H	-0.192600	-4.577254	3.344525
H	1.473397	-5.045902	3.713381
H	0.854173	-3.481480	4.263645
H	-4.766074	2.195442	-1.864153
H	-6.284015	1.492830	-1.283181
H	-5.260101	2.422058	-0.177421
H	-3.481000	0.809288	-3.250012
H	-4.641871	-0.496348	-3.538976
H	-2.914628	-0.858795	-3.431980
H	-5.147843	1.510474	1.910796
H	-6.144304	0.050758	2.013271
H	-4.576973	0.109516	2.834886

$[Ni(GaCp^*)_3(C_2H_4)]$:

Ni	0.327131	0.611410	-0.540698
C	0.034266	0.060394	-2.467788
C	0.879672	1.178174	-2.396548
H	-1.020976	0.174968	-2.719129
H	0.448917	-0.929664	-2.660339
H	0.494117	2.181950	-2.580552
H	1.957374	1.061990	-2.520376
Ga	0.261985	-1.413497	0.491069
C	0.367448	-3.614414	-0.497195
C	-0.062076	-3.714070	0.867207
C	-1.348221	-4.311904	1.348046
H	-1.652270	-3.899097	2.318859
H	-1.255149	-5.402878	1.474076
H	-2.171283	-4.137178	0.642580
C	1.021668	-3.269054	1.705903
C	2.109137	-2.897613	0.851529
C	1.700794	-3.104523	-0.502840
C	2.546012	-2.803173	-1.701624
H	2.999351	-1.803510	-1.632778
H	3.368177	-3.528666	-1.807010
H	1.960515	-2.838065	-2.628799
C	-0.439775	-4.004361	-1.697124
H	-1.515425	-3.872255	-1.522035
H	-0.280488	-5.061756	-1.962296
H	-0.175588	-3.404192	-2.577654
C	1.025003	-3.301563	3.203710
H	0.048441	-3.019492	3.620993
H	1.772901	-2.615986	3.622267
H	1.260186	-4.309305	3.582002
C	3.450228	-2.375209	1.265032
H	3.515313	-2.245392	2.351377
H	3.668237	-1.400441	0.800450
H	4.254884	-3.064290	0.965692

Ga	1.680233	1.637719	0.975312
C	0.947842	3.237845	2.654717
C	2.232906	3.618439	2.157174
C	2.573340	4.902111	1.463807
H	3.412864	4.775968	0.767349
H	2.863913	5.682422	2.185389
H	1.723291	5.290316	0.887579
C	3.163999	2.575440	2.495190
C	2.440258	1.556011	3.206760
C	1.073804	1.963962	3.291476
C	-0.054957	1.181210	3.885524
H	0.211041	0.123934	4.012990
H	-0.351806	1.571170	4.871854
H	-0.942716	1.217759	3.236406
C	-0.325732	4.010081	2.527888
H	-0.229404	4.839792	1.816752
H	-0.639021	4.432279	3.495355
H	-1.148858	3.368094	2.171421
Ga	-1.691413	1.417298	0.283781
C	-3.899362	1.092024	-0.653672
C	-4.000862	2.082697	0.376082
C	-4.424616	3.507891	0.193622
H	-3.965238	4.167362	0.942635
H	-5.517068	3.619546	0.290177
H	-4.147254	3.890202	-0.797972
C	-3.709902	1.448495	1.630846
C	-3.804127	2.103591	2.974803
H	-3.474265	3.151092	2.943536
H	-3.191079	1.589335	3.726246
H	-4.841743	2.103666	3.346325
C	-3.425284	0.070927	1.370245
C	-3.060918	-0.979800	2.371703
H	-2.877876	-0.549339	3.364208
H	-2.144905	-1.517723	2.073391
H	-3.855340	-1.734923	2.478074
C	-3.542678	-0.147231	-0.037764
C	-3.316956	-1.456585	-0.724786
H	-2.446462	-1.980289	-0.301114
H	-4.185577	-2.127049	-0.622694
H	-3.123913	-1.325766	-1.797086
C	-4.159389	1.313151	-2.112674
H	-3.879784	2.328120	-2.425996
H	-5.225161	1.179312	-2.358827
H	-3.592701	0.608983	-2.736529
C	4.644539	2.607742	2.267607
H	5.166460	3.093303	3.108030
H	4.904371	3.166275	1.358635
H	5.062685	1.597450	2.165988
C	3.032264	0.325836	3.819068
H	3.930326	-0.004507	3.282154
H	2.318161	-0.508430	3.816517
H	3.323039	0.502108	4.867014

$[Ni(GaCp^*)_3(C_2H_2)]$:

Ga	-1.757547	1.332707	0.341842
Ga	1.641039	1.776386	0.854139
Ga	0.353032	-1.290696	0.779122
Ni	0.247535	0.680126	-0.578077
C	2.802756	0.240520	3.681561
C	4.624494	2.467853	2.231191
C	-4.138973	1.150254	-2.106055
C	-3.370940	-1.562730	-0.534807
C	-3.594834	-0.209347	0.061138
C	-3.155545	-0.910892	2.520294
C	-3.479772	0.090190	1.455375
C	-3.839247	2.225733	2.929127
C	-3.722752	1.490834	1.629538
C	-4.368318	3.477823	0.055731
C	-3.978145	2.057794	0.330347
C	-3.907279	0.999085	-0.633614
C	-0.255953	4.179255	2.418660
C	-0.158915	1.296924	3.764617
C	1.003318	2.039016	3.186195
C	2.339693	1.544552	3.113392
C	3.140971	2.523484	2.434590
C	2.724826	4.915711	1.460030
C	2.282314	3.634144	2.098230
C	0.964996	3.327148	2.569830
C	3.589354	-2.457986	1.398704
C	1.209957	-3.639809	3.230943
C	-0.359777	-3.605038	-1.693788
C	2.595864	-2.433754	-1.591866
C	1.778242	-2.861650	-0.414059
C	2.222313	-2.868650	0.944723
C	1.168032	-3.399800	1.752770
C	-1.205553	-4.381439	1.315917
C	0.071683	-3.725758	0.887783
C	0.451916	-3.393507	-0.452372
C	0.942175	0.430083	-2.360269
C	-0.304109	0.189165	-2.361627
H	1.894702	0.509575	-2.863242
H	-1.213312	-0.088192	-2.874811
H	2.908195	0.299584	4.776463
H	2.087440	-0.566738	3.465031
H	3.774597	-0.059145	3.272171
H	4.982504	1.434349	2.135858
H	4.932669	3.009654	1.327237
H	5.158664	2.921977	3.081173
H	-3.706309	0.314021	-2.669696
H	-5.214474	1.179245	-2.342144
H	-3.694432	2.075764	-2.496696
H	-3.288942	-1.518436	-1.627514
H	-4.192929	-2.253630	-0.290788
H	-2.440451	-2.010307	-0.154558

H	-4.003391	-1.587951	2.708483
H	-2.296285	-1.537198	2.231446
H	-2.901763	-0.425042	3.470501
H	-4.894938	2.329204	3.227273
H	-3.323677	1.700063	3.742490
H	-3.420999	3.240118	2.870258
H	-4.065138	3.793558	-0.951294
H	-5.460166	3.612159	0.124193
H	-3.910704	4.171640	0.773638
H	-1.110189	3.592104	2.042508
H	-0.561247	4.623006	3.378690
H	-0.090391	5.000497	1.710512
H	-1.108788	1.748005	3.453920
H	-0.135508	1.294248	4.865678
H	-0.168720	0.246796	3.431934
H	1.916586	5.383784	0.883092
H	3.052256	5.645459	2.217807
H	3.568801	4.757741	0.775683
H	4.349062	-3.193103	1.087955
H	3.887320	-1.488028	0.972482
H	3.645250	-2.373177	2.490549
H	1.507396	-4.675059	3.465475
H	1.928243	-2.976269	3.731022
H	0.228799	-3.473367	3.697484
H	-0.251005	-2.762359	-2.390703
H	-0.048258	-4.517264	-2.227702
H	-1.428101	-3.711429	-1.466587
H	1.958750	-2.153583	-2.439518
H	3.266788	-3.241002	-1.929270
H	3.223516	-1.564142	-1.351729
H	-2.024619	-4.179510	0.613217
H	-1.094279	-5.476500	1.376930
H	-1.529463	-4.036059	2.307858

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