

Supplementary Information

Suppressed Phosphine Dissociation by Polarization Effects on the Donor-Acceptor Bonds in $[\text{Ni}(\text{PEt}_3)_{4-n}(\text{ECp}^*)_n]$ (E = Al, Ga).

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Experimental Spectra

^1H , ^{13}C , ^{27}Al , ^{31}P -NMR and IR-Spectra of $[\text{Ni}(\text{ECp}^*)_n(\text{PEt}_3)_{4-n}]$

Table S 1: Overview of the $^1\text{H}/^{13}\text{C}/^{27}\text{Al}/^{31}\text{P}$ chemical shifts of **1a -5** (C_6D_6 , 298K).

Compound	^1H -NMR	^{13}C -NMR	^{31}P - NMR	^{27}Al -NMR
$\text{Ni}(\text{PEt}_3)_4$	1.60 (m, 24 H), 0.94 (m, 36H)		17.8	
$\text{Ni}(\text{GaCp}^*)(\text{PEt}_3)_3$	2.14 (s, 15H), 1.36 (m, 18H), 1.03 (m, 27H)	113.0, 23.1, 10.8, 8.9	16.6	
$\text{Ni}(\text{GaCp}^*)_2(\text{PEt}_3)_2$	2.07 (s, 30H), 1.22 (m, 12H), 0.97 (m, 18H)	112.9, 26.4, 10.4, 9.4	29.4	
$\text{Ni}(\text{GaCp}^*)_3(\text{PEt}_3)$ (could never be isolated in pure form)	2.01 (s, 45H), 1.09 (m, 6H), 0.95 (m, 9H)		45.7	
$\text{Ni}(\text{GaCp}^*)_4$	1.94 (s, 60H)			
$\text{Ni}(\text{AlCp}^*)(\text{PEt}_3)_3$	2.04 (s, 15H), 1.43 (m, 18H), 1.07 (m, 27H)	113.5, 25.9, 10.7, 9.1	19.5	-71.2
$\text{Ni}(\text{AlCp}^*)_2(\text{PEt}_3)_2$	2.01 (s, 30H), 1.26 (m, 12H), 1.03 (m, 18H)	113.3, 28.4, 10.7, 9.7	39.4	-61.3
$\text{Ni}(\text{AlCp}^*)_3(\text{PEt}_3)$	1.98 (s, 45H), 1.05 (m, 6H), 0.99 (m, 9H)	112.8, 29.0, 10.4, 10.3	61.9	-53.1
$\text{Ni}(\text{AlCp}^*)_4$	1.93 (s, 60H)			

1a Ni(AlCp*)₁(PEt₃)₃:

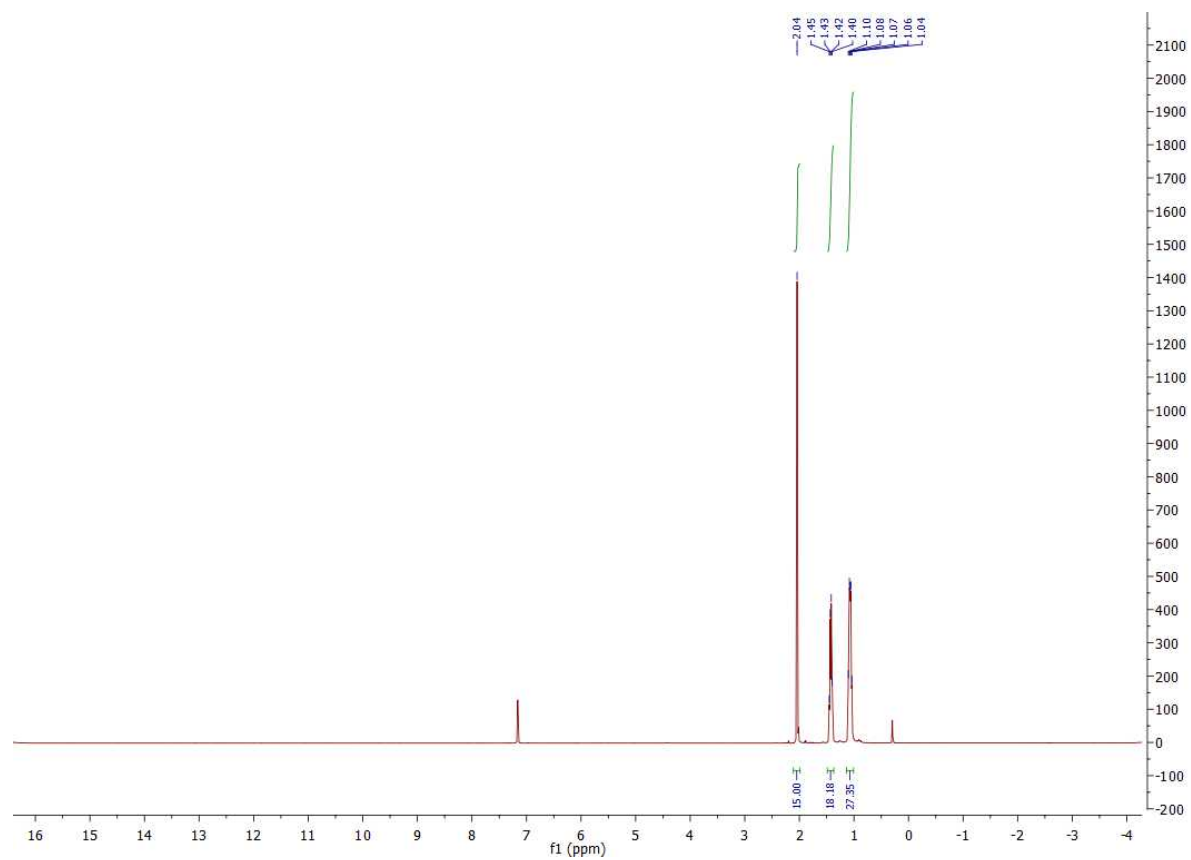


Figure S 1: ¹H-NMR of **1a** (400 MHz, C₆D₆).

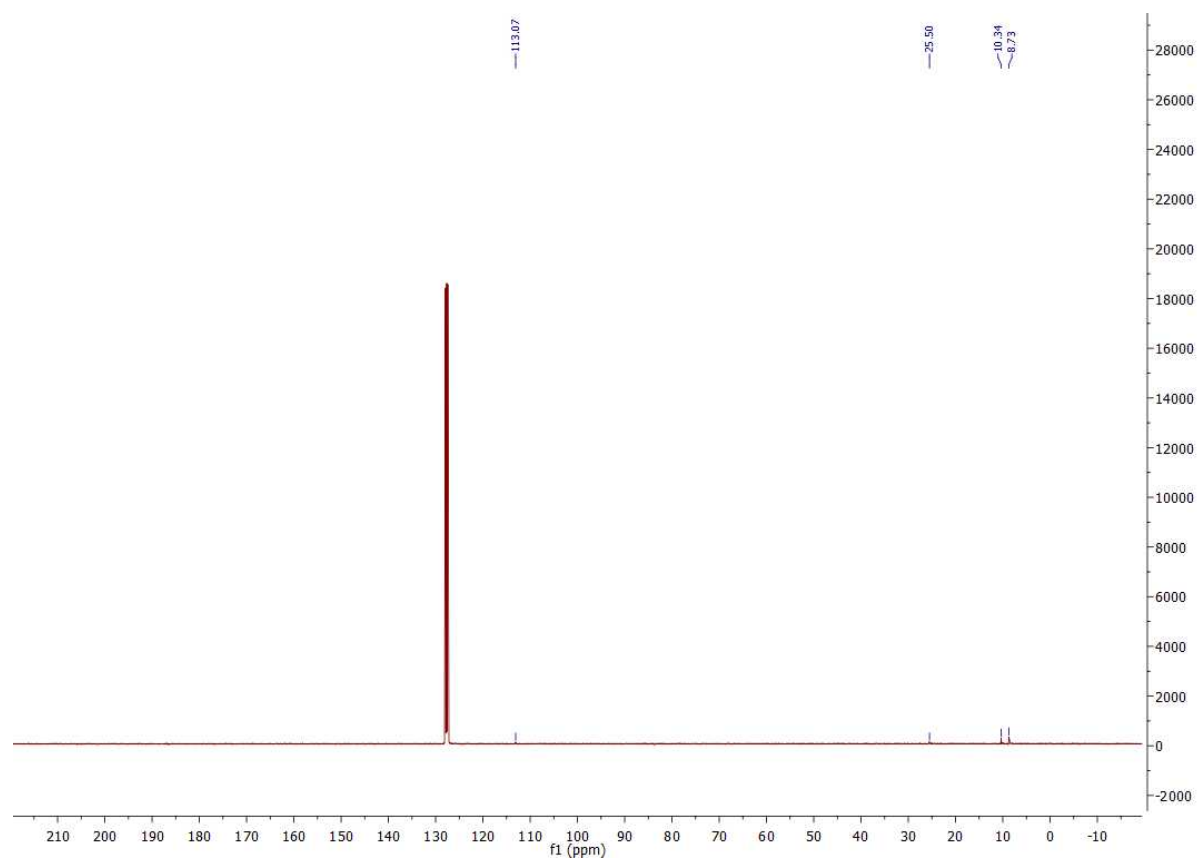


Figure S 2: ^{13}C -NMR of **1a** (100 MHz, C_6D_6).

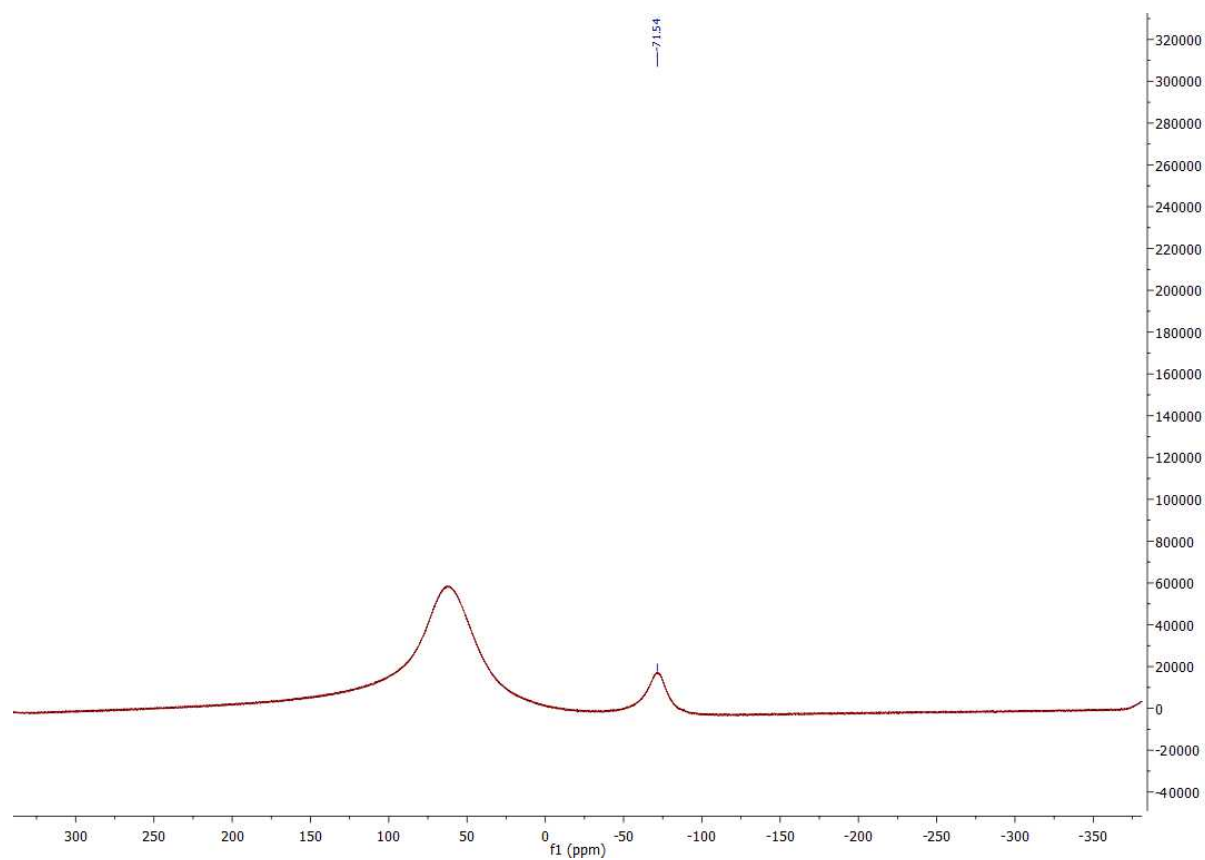


Figure S 3: ^{27}Al -NMR of **1a** (104 MHz, C_6D_6).

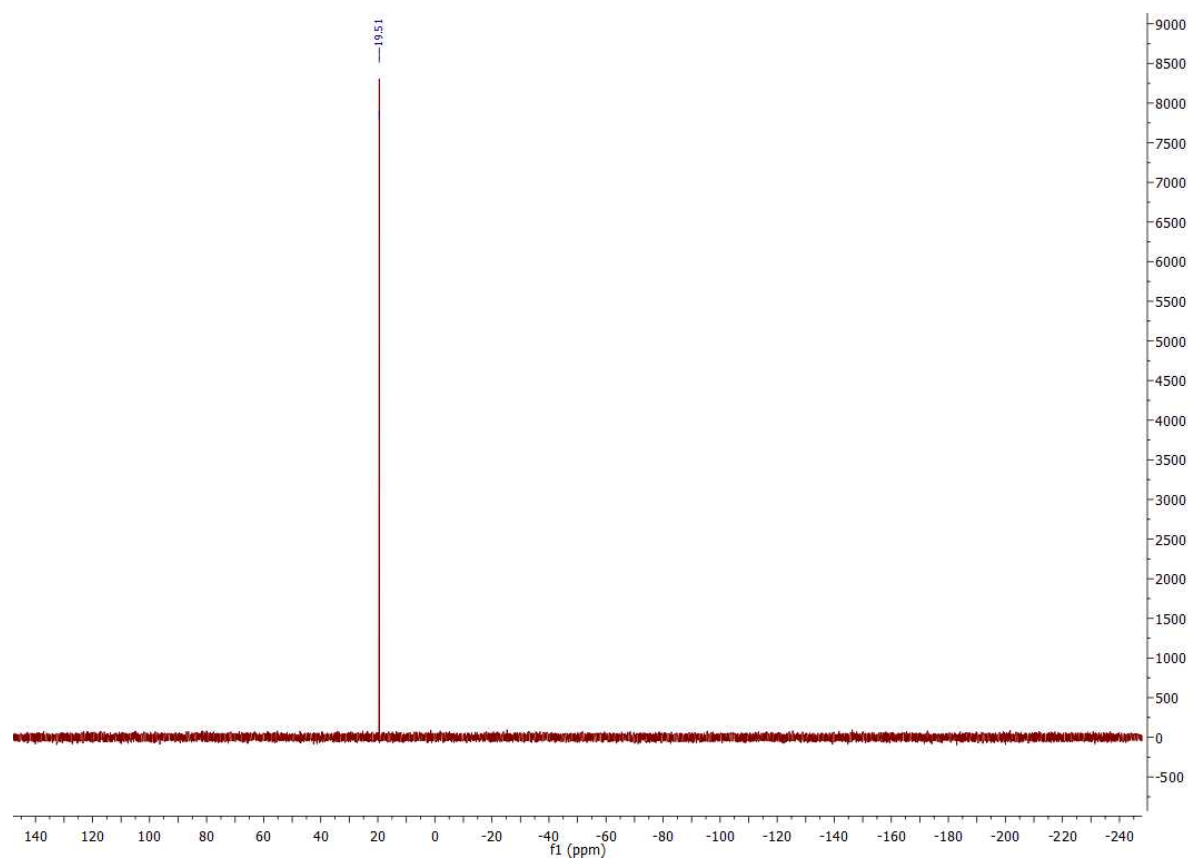


Figure S 4: ^{31}P -NMR of **1a** (162 MHz, C_6D_6).

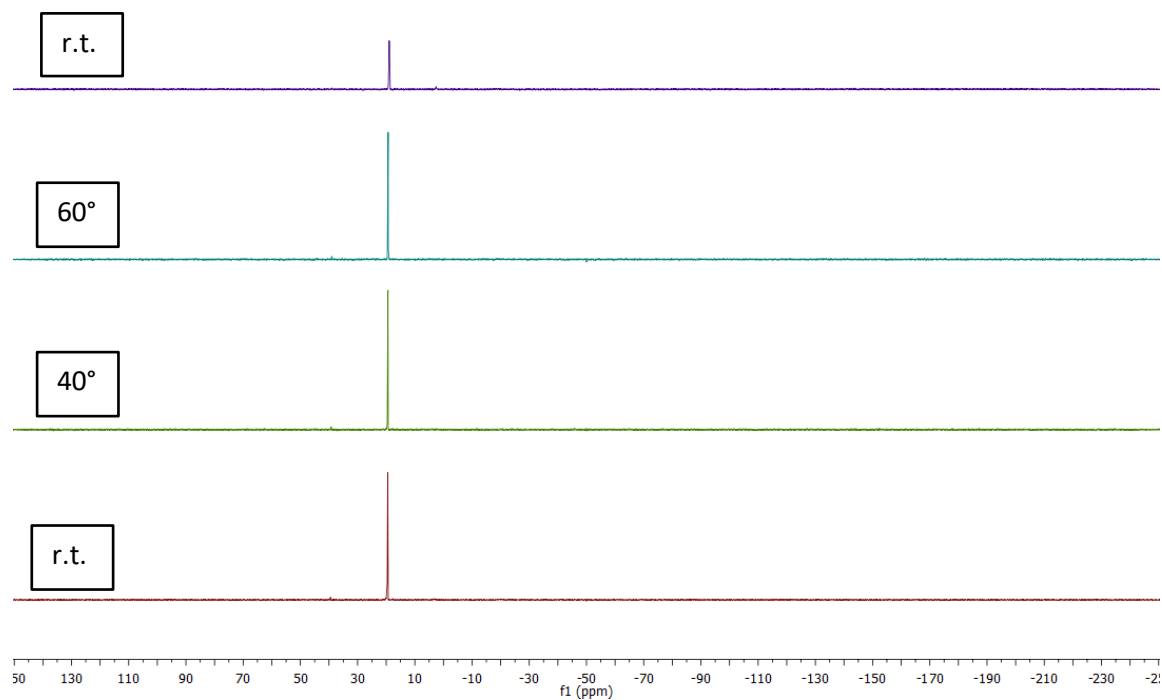


Figure S 5: ^{31}P VT- NMR of **1a** (162 MHz, Toluene- d_6)

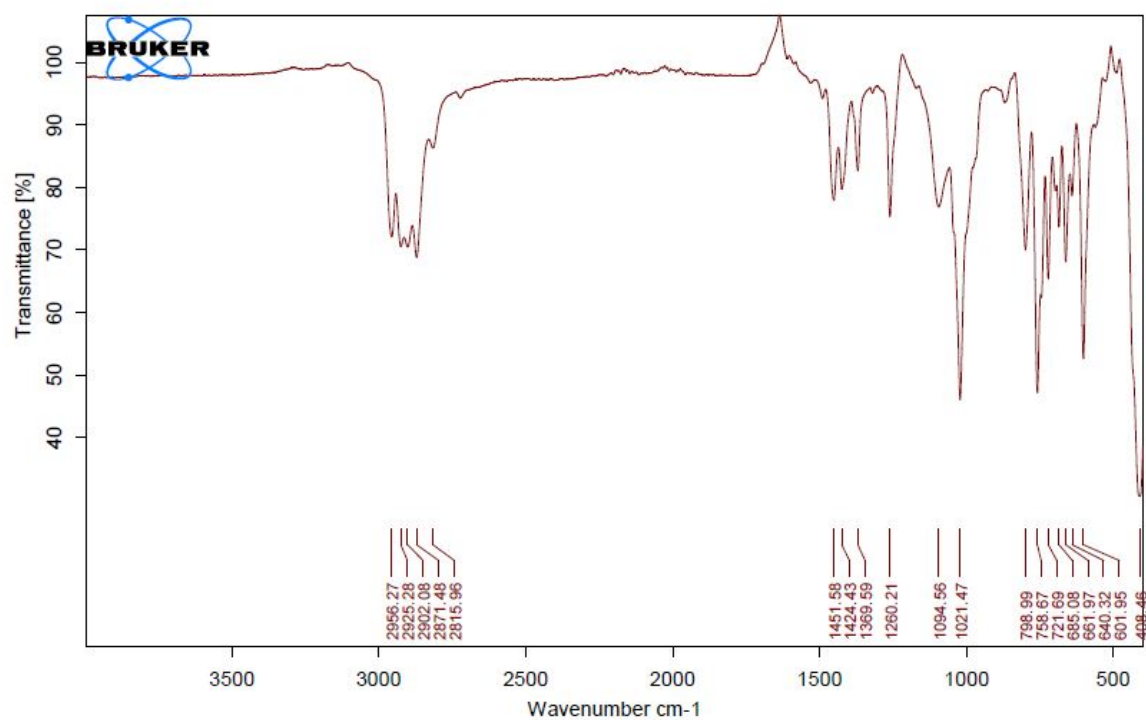


Figure S 6: IR-Spectrum of **1a**.

2a Ni(AlCp*)₂(PEt₃)₂:

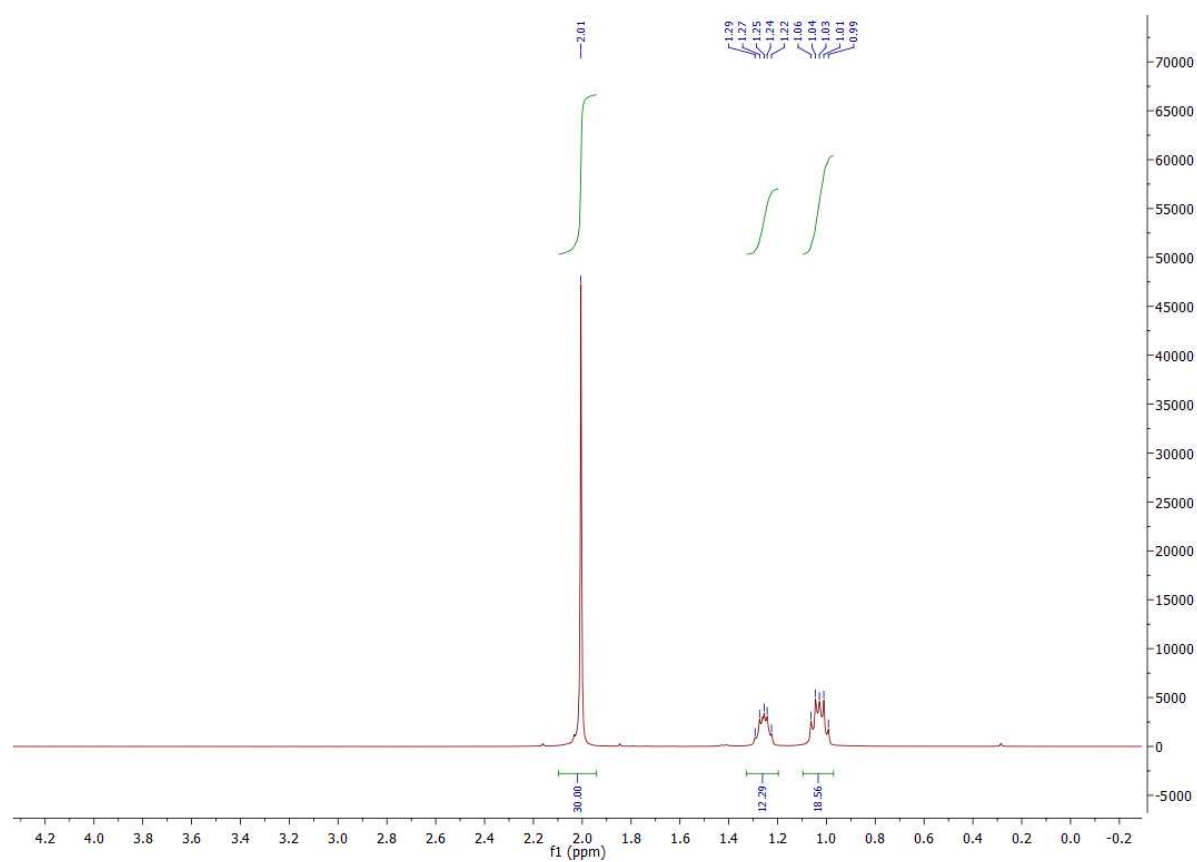


Figure S 7: ¹H-NMR of **2a** (400 MHz, C₆D₆).

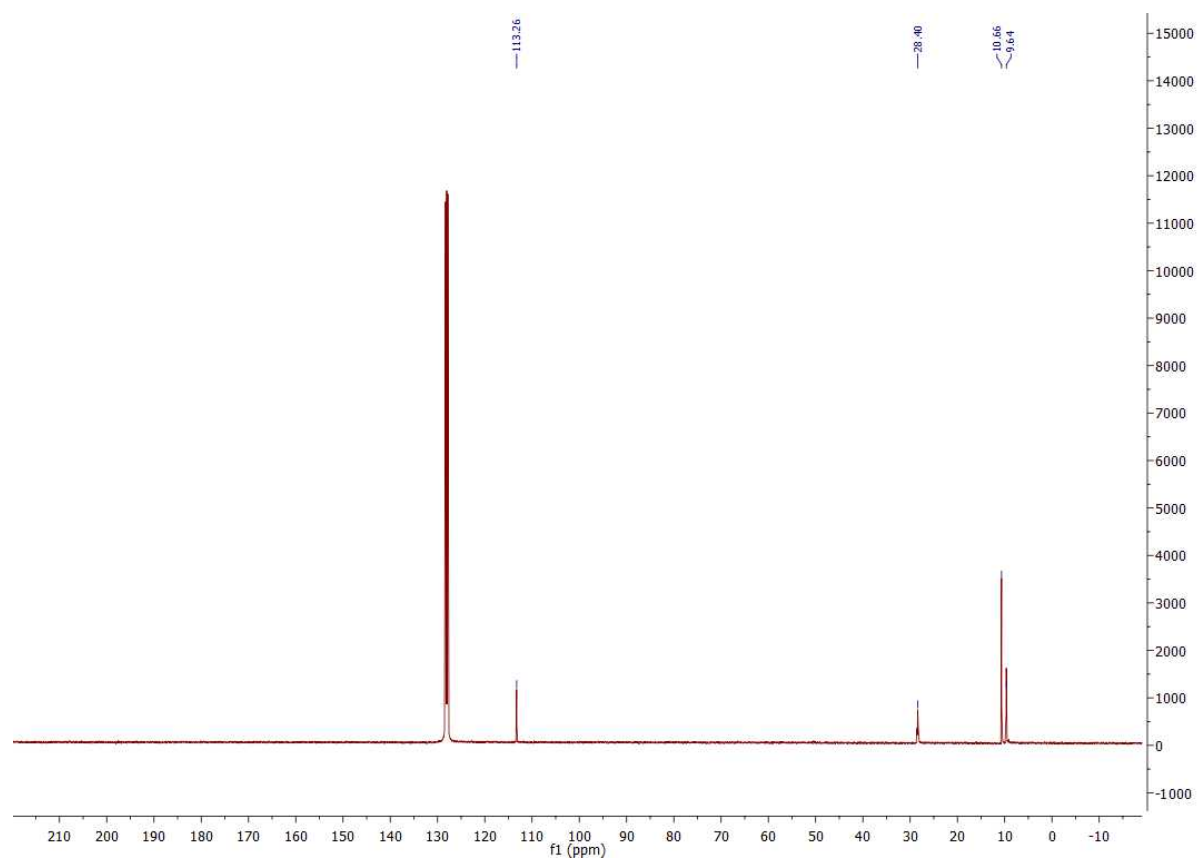


Figure S 8: ^{13}C -NMR of **2a** (100 MHz, C_6D_6).

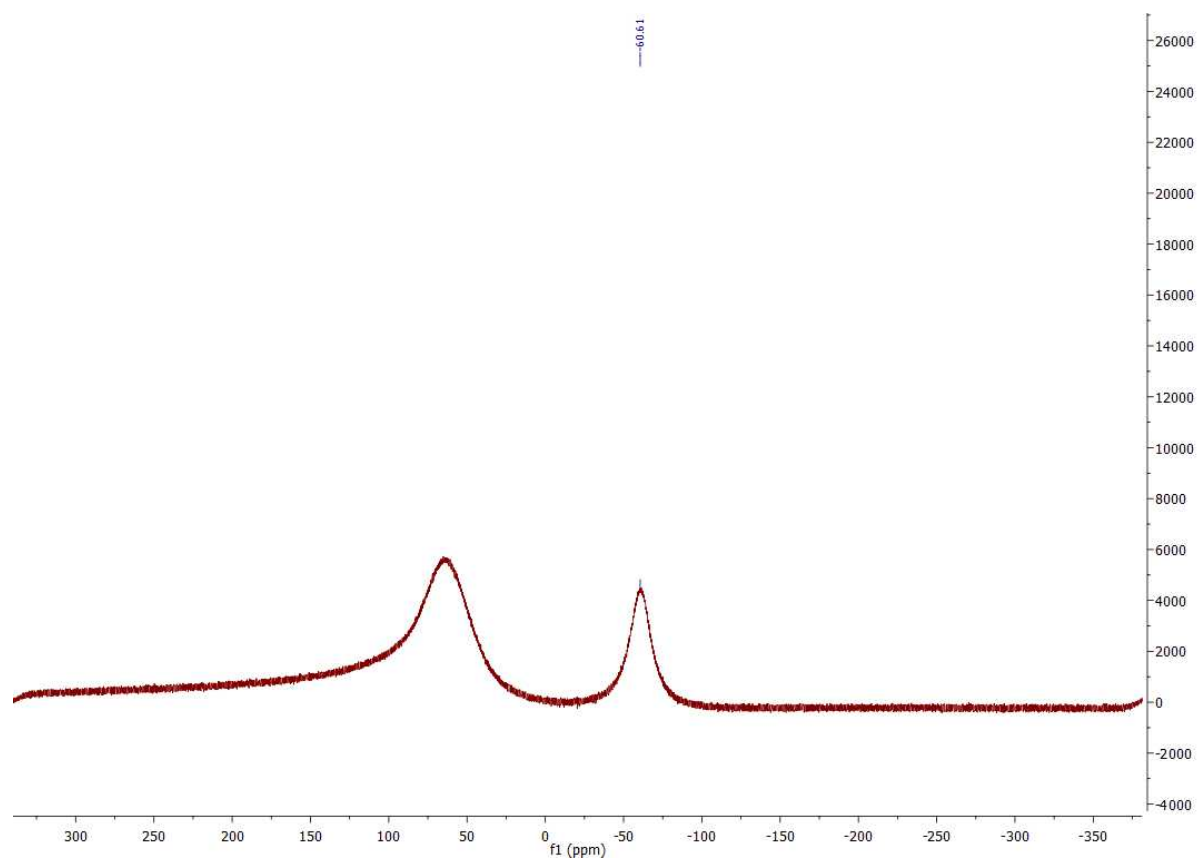


Figure S 9: ^{27}Al -NMR of **2a** (104 MHz, C_6D_6).

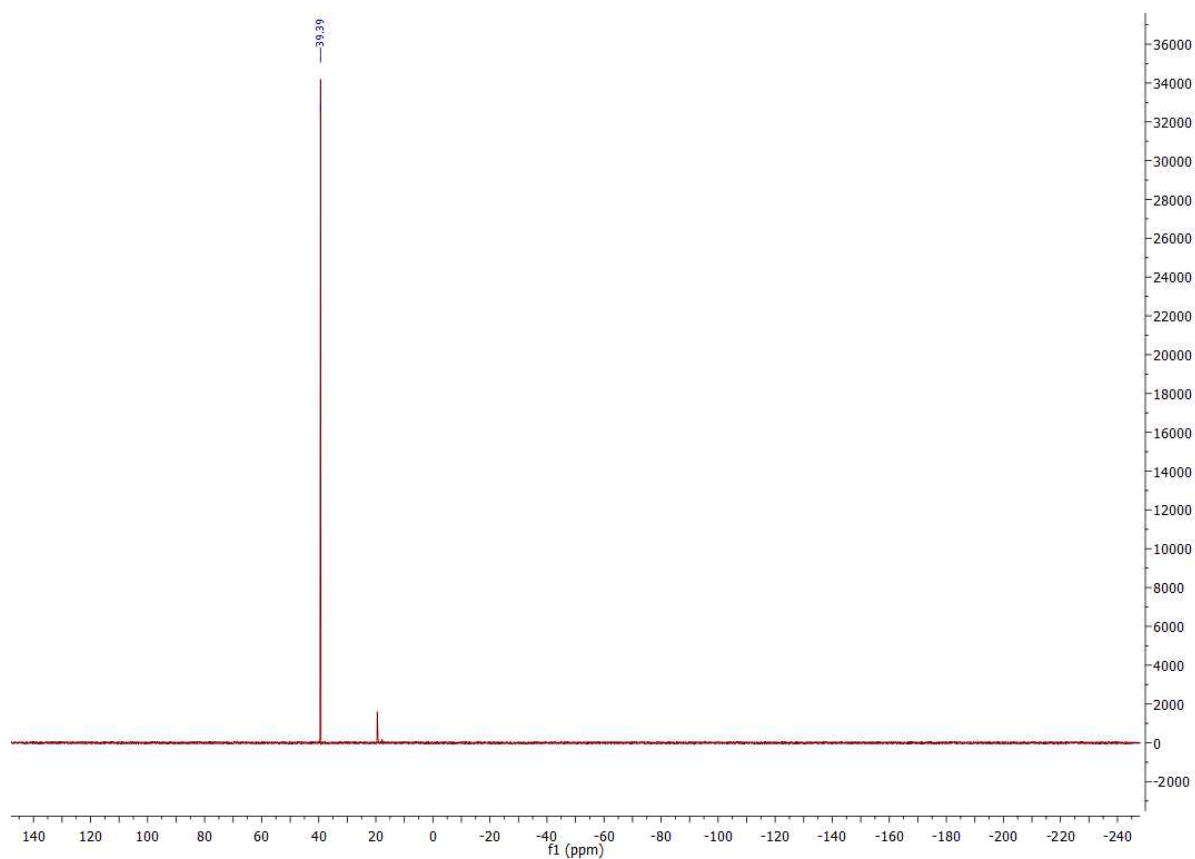


Figure S 10: ^{31}P -NMR of **2a** (162 MHz, C_6D_6).

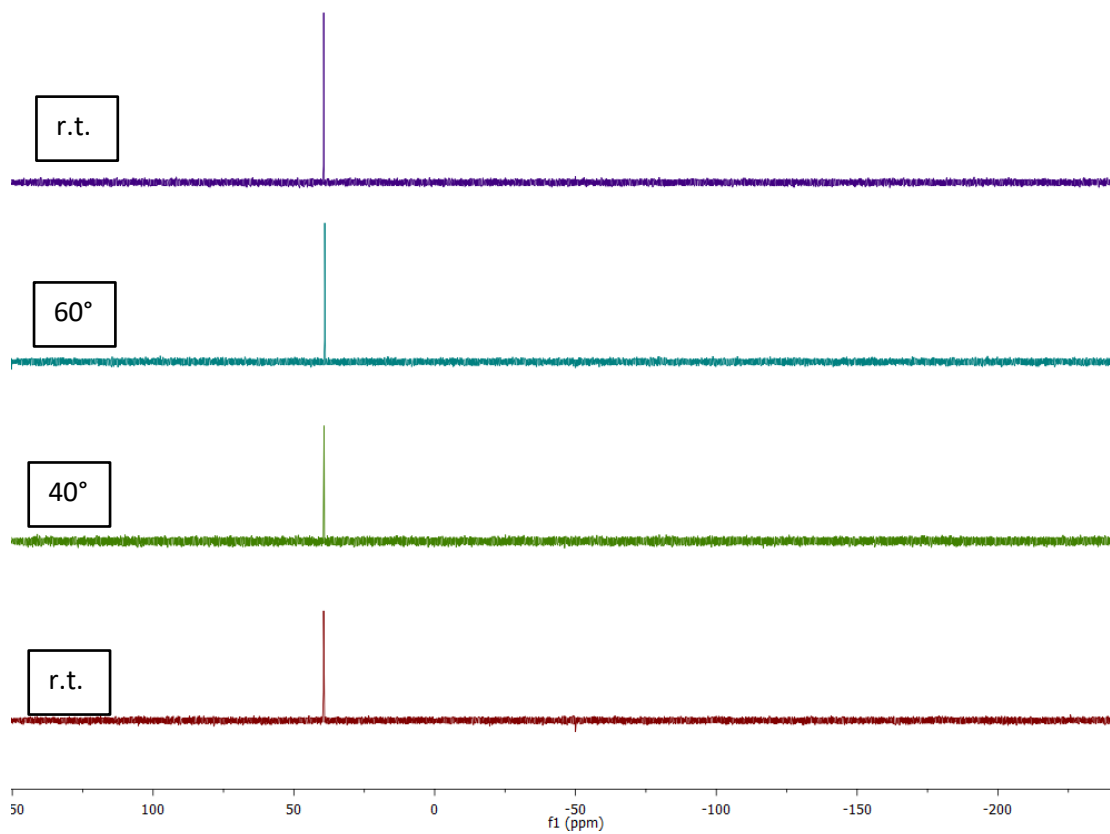


Figure S 11: ^{31}P VT-NMR of **2a** (162 MHz, Toluene- d_6).

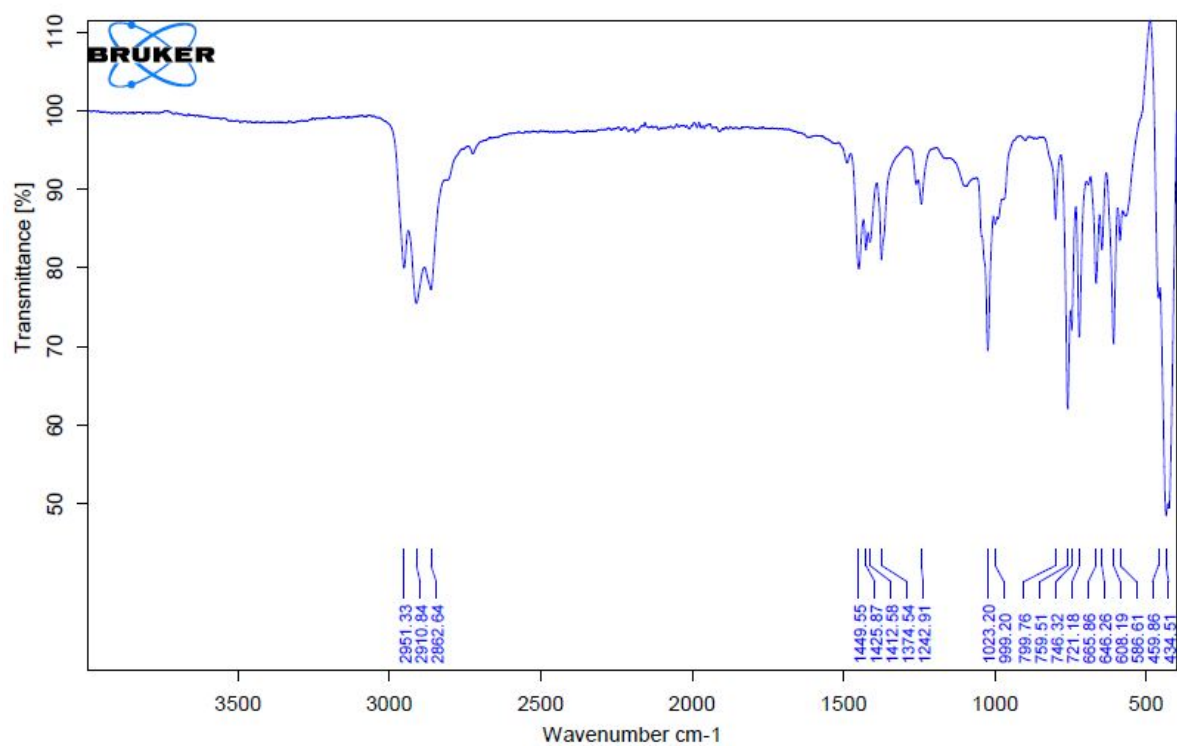


Figure S 12: IR-Spectrum of **2a**.

3a Ni(AlCp*)₃(PEt₃):

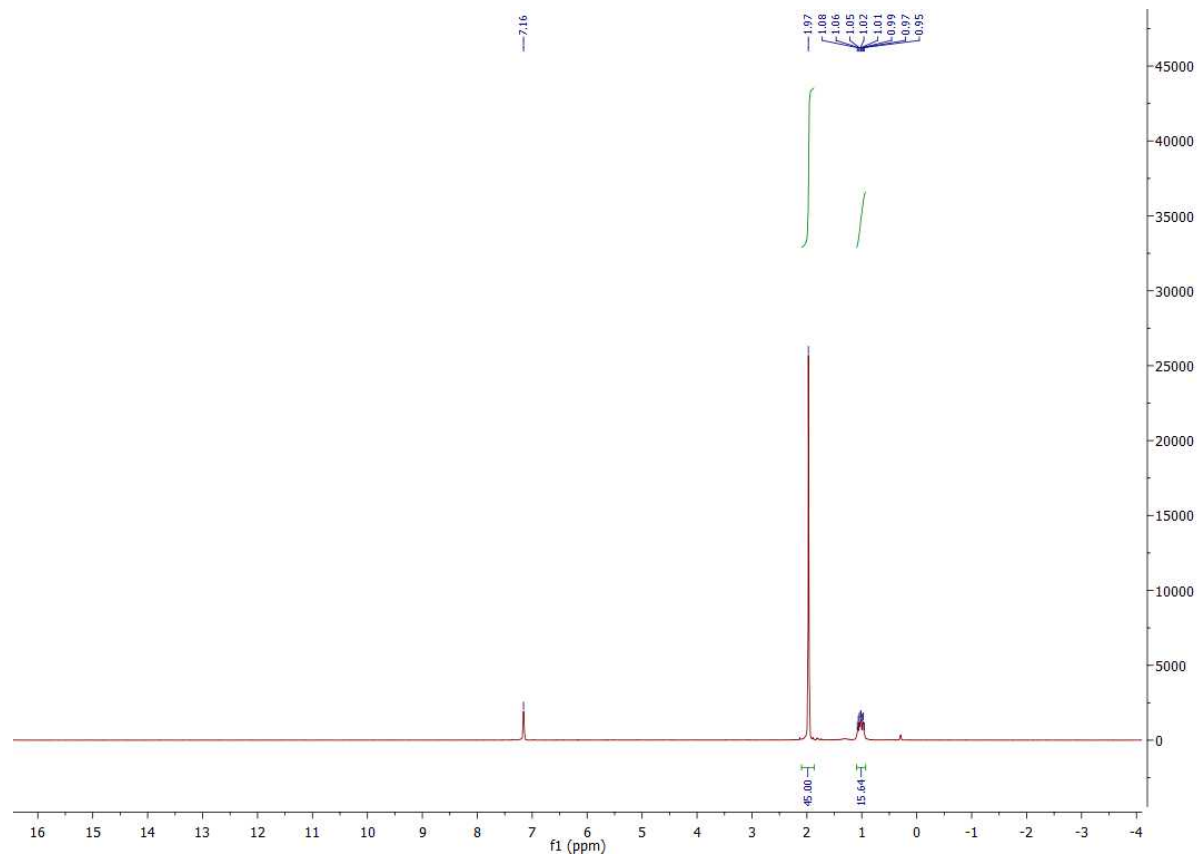


Figure S 13: ¹H-NMR of **3a** (400 MHz, C₆D₆).

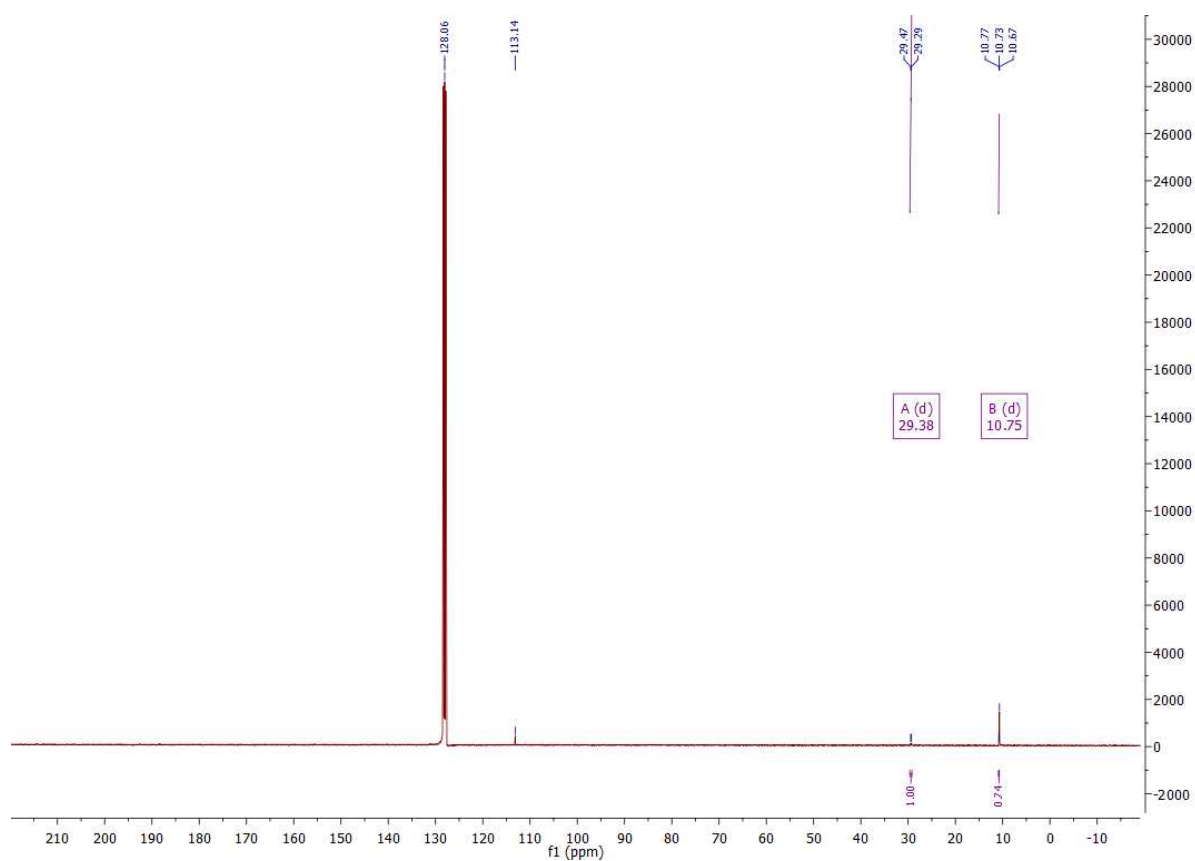


Figure S 14: ¹³C-NMR of **3a** (100 MHz, C₆D₆).

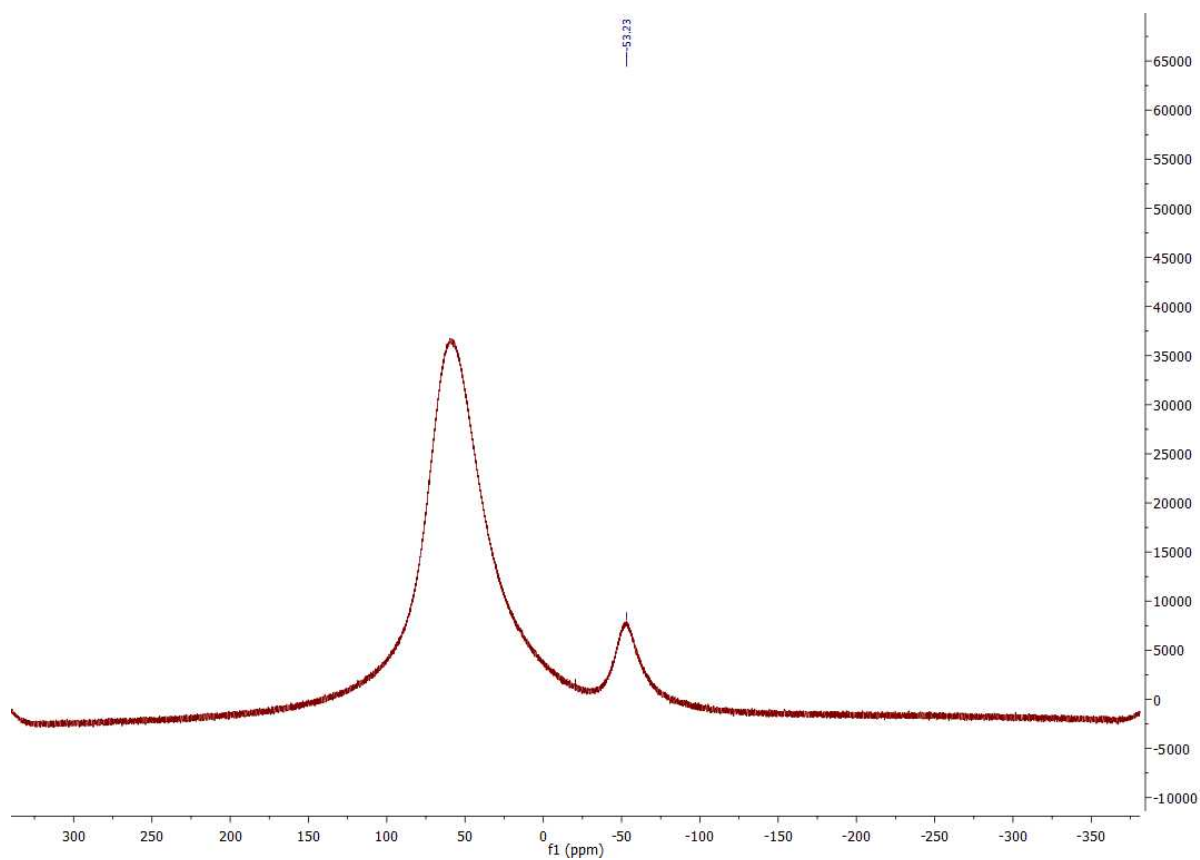


Figure S 15: ²⁷Al-NMR of **3a** (104 MHz, C₆D₆).

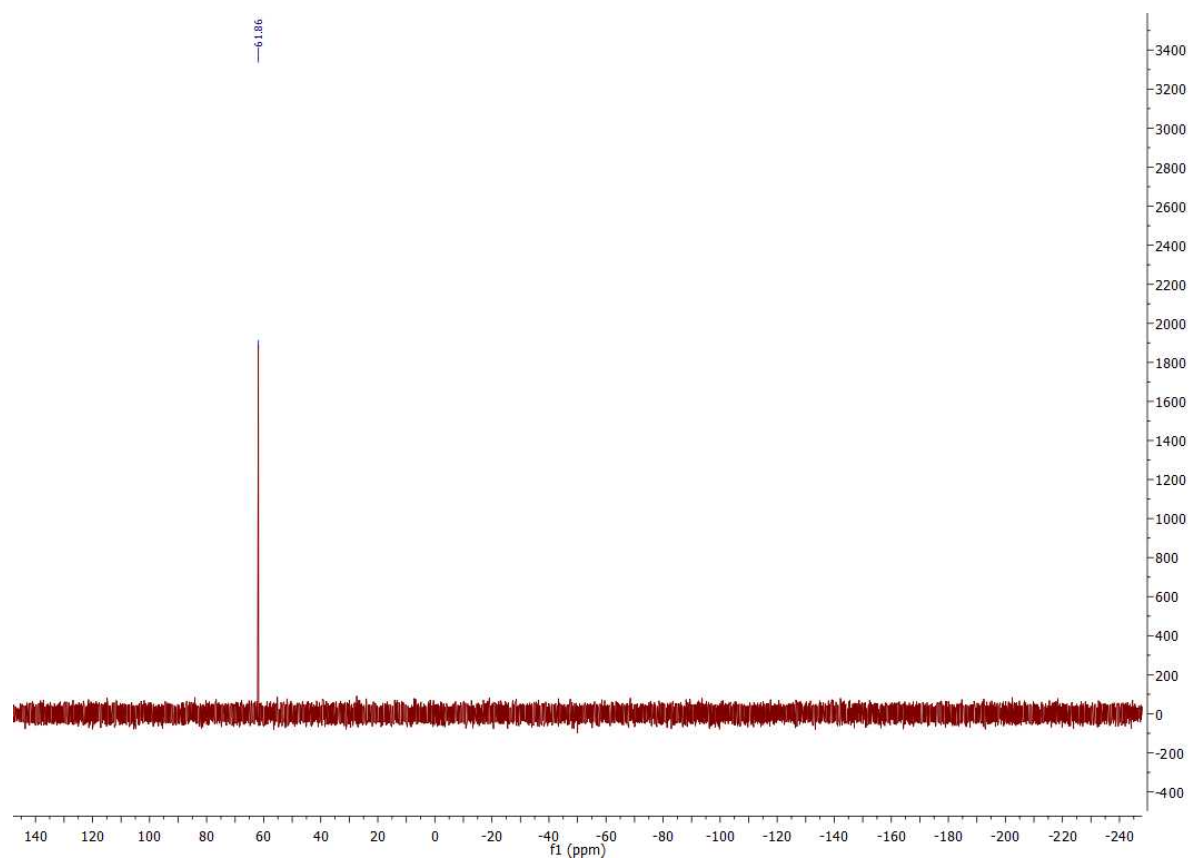


Figure S 16: ^{31}P -NMR of **3a** (162 MHz, C_6D_6).

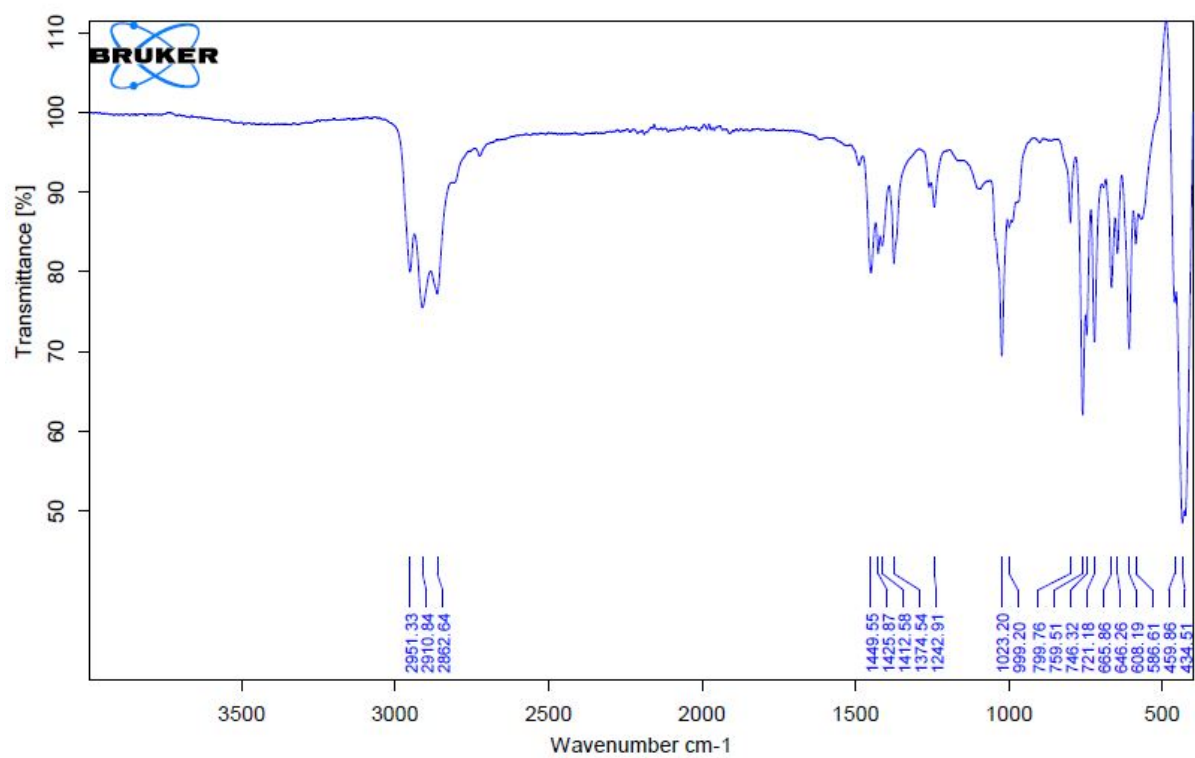


Figure S 17: IR Spectrum of **3a**.

1b Ni(GaCp*)(PEt₃)₃:

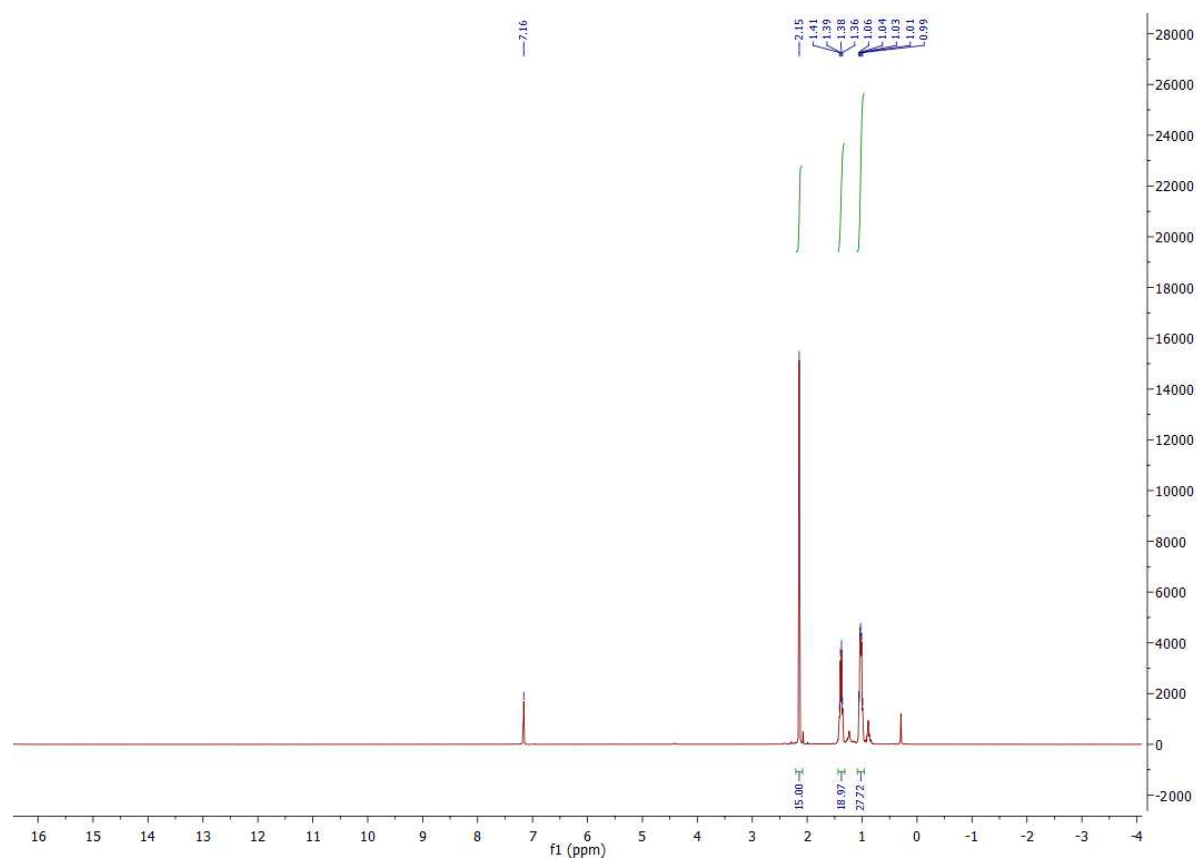


Figure S 18: ¹H-NMR of **1b** (400 MHz, C₆D₆).

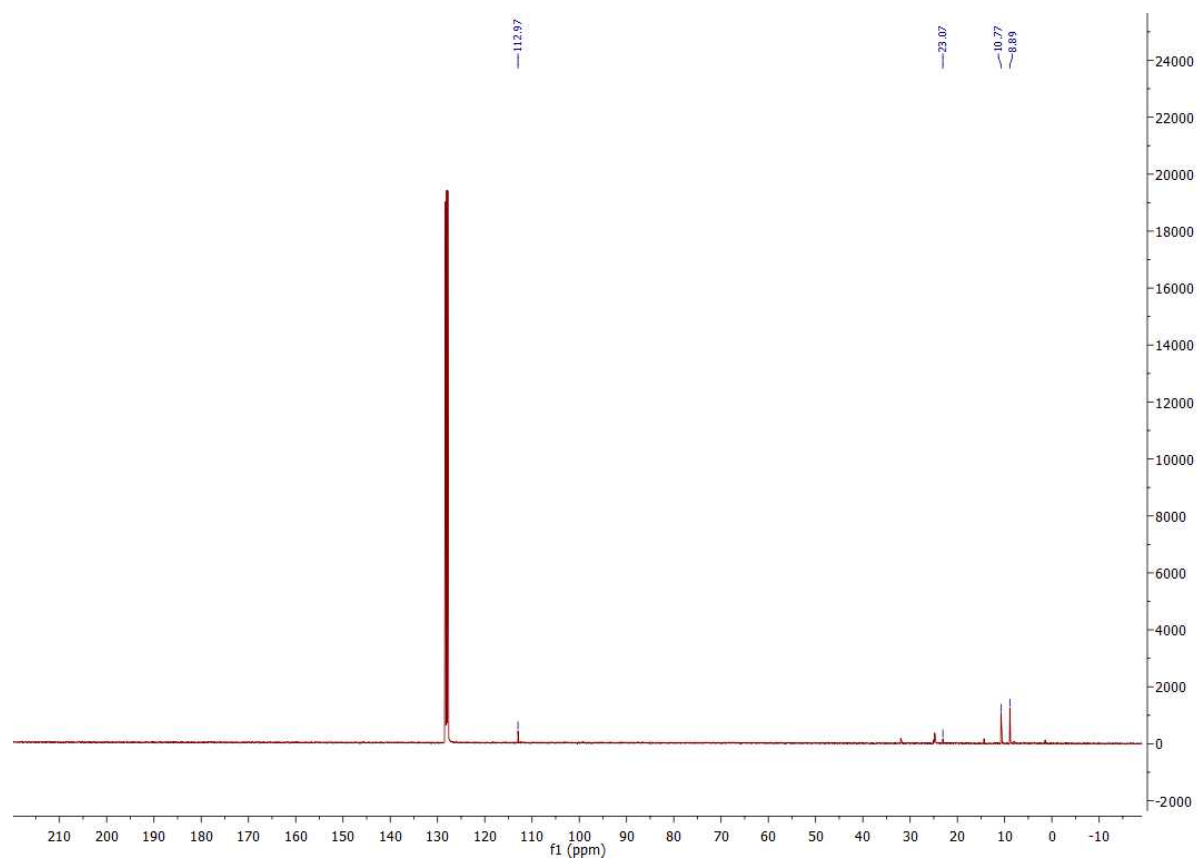


Figure S 19: ^{13}C -NMR of **1b** (100 MHz, C_6D_6).

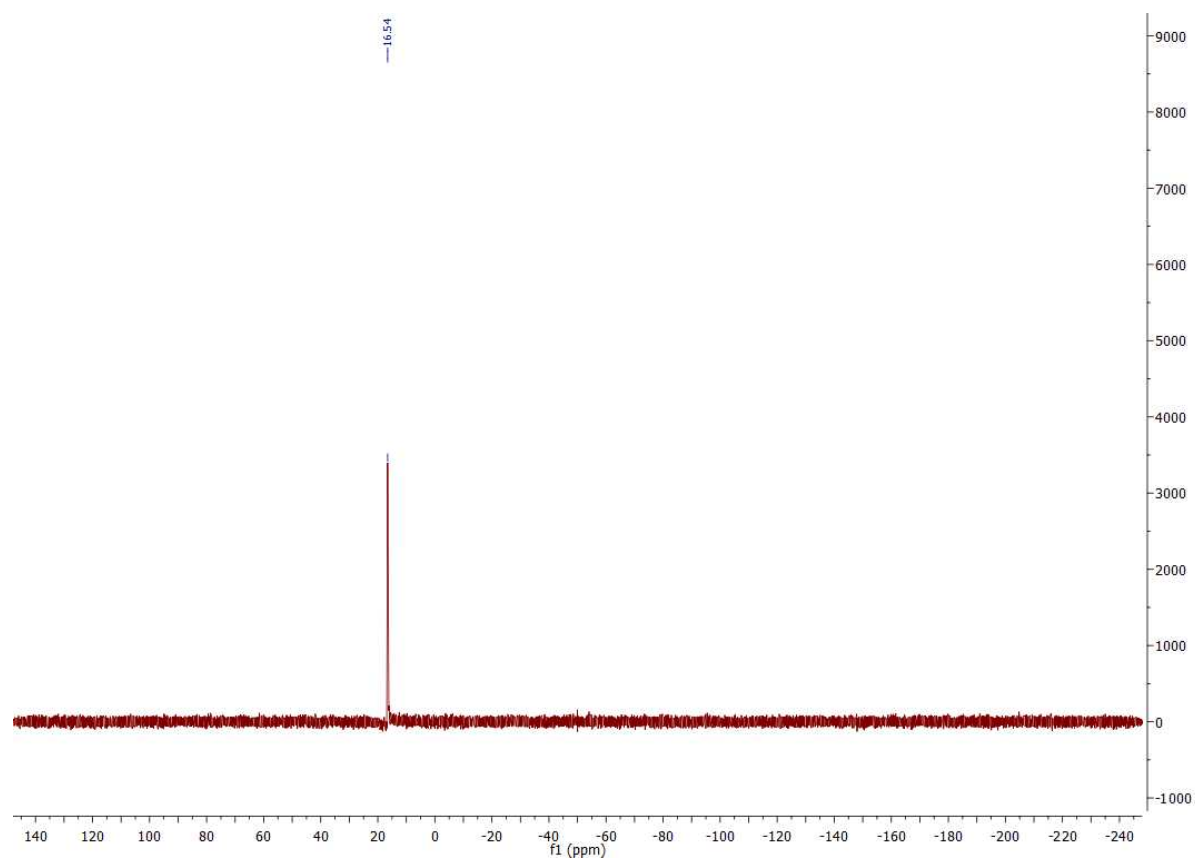


Figure S 20: ^{31}P -NMR of **1b** (162 MHz, C_6D_6).

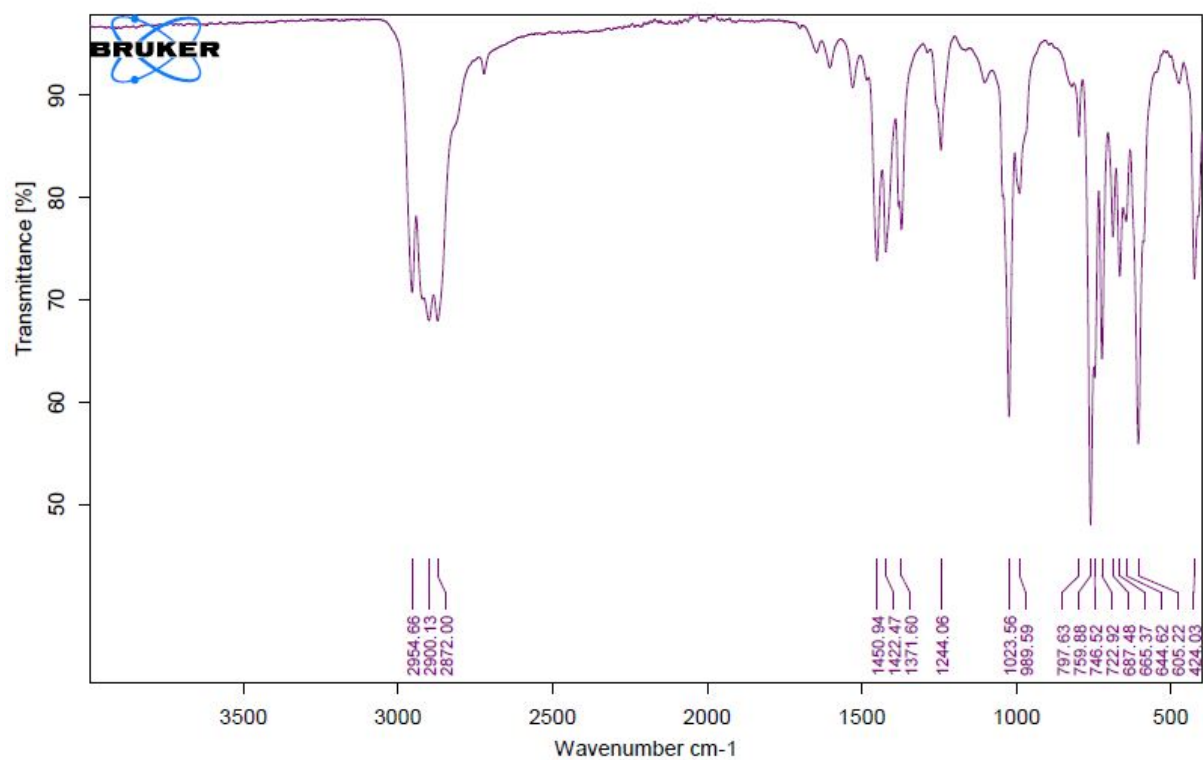


Figure S 21: IR Spectrum of **1b**.

2b Ni(GaCp*)₂(PEt₃)₂:

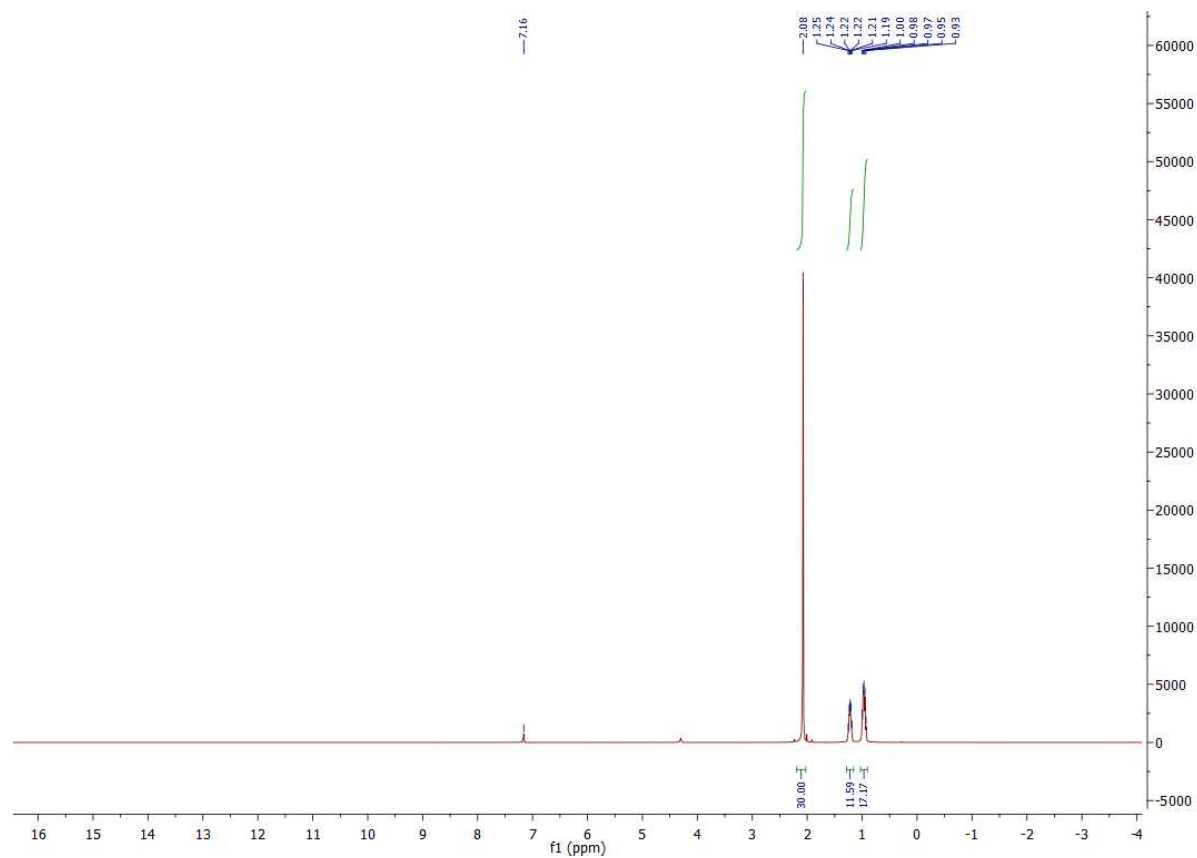


Figure S 22: ¹H-NMR of **2b** (400 MHz, C₆D₆).

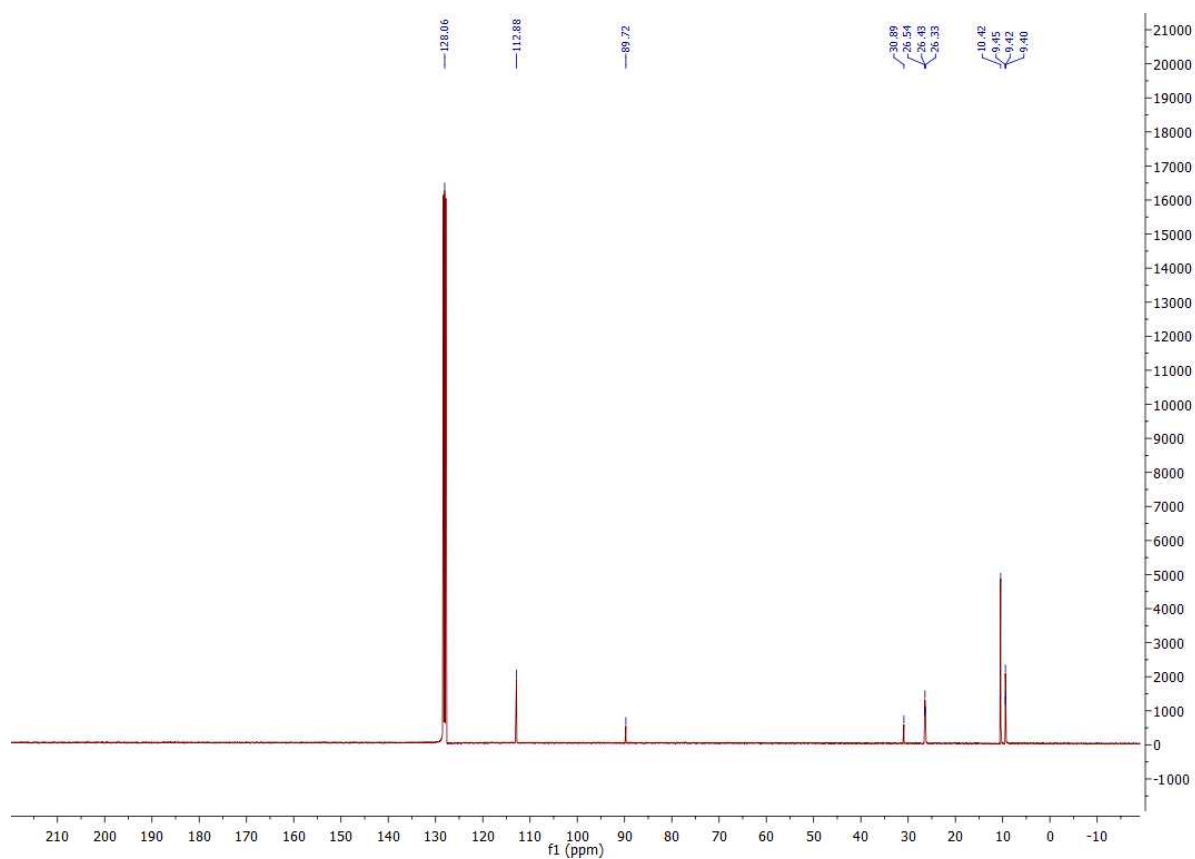


Figure S 23: ^{13}C -NMR of **2b** (100 MHz, C_6D_6).

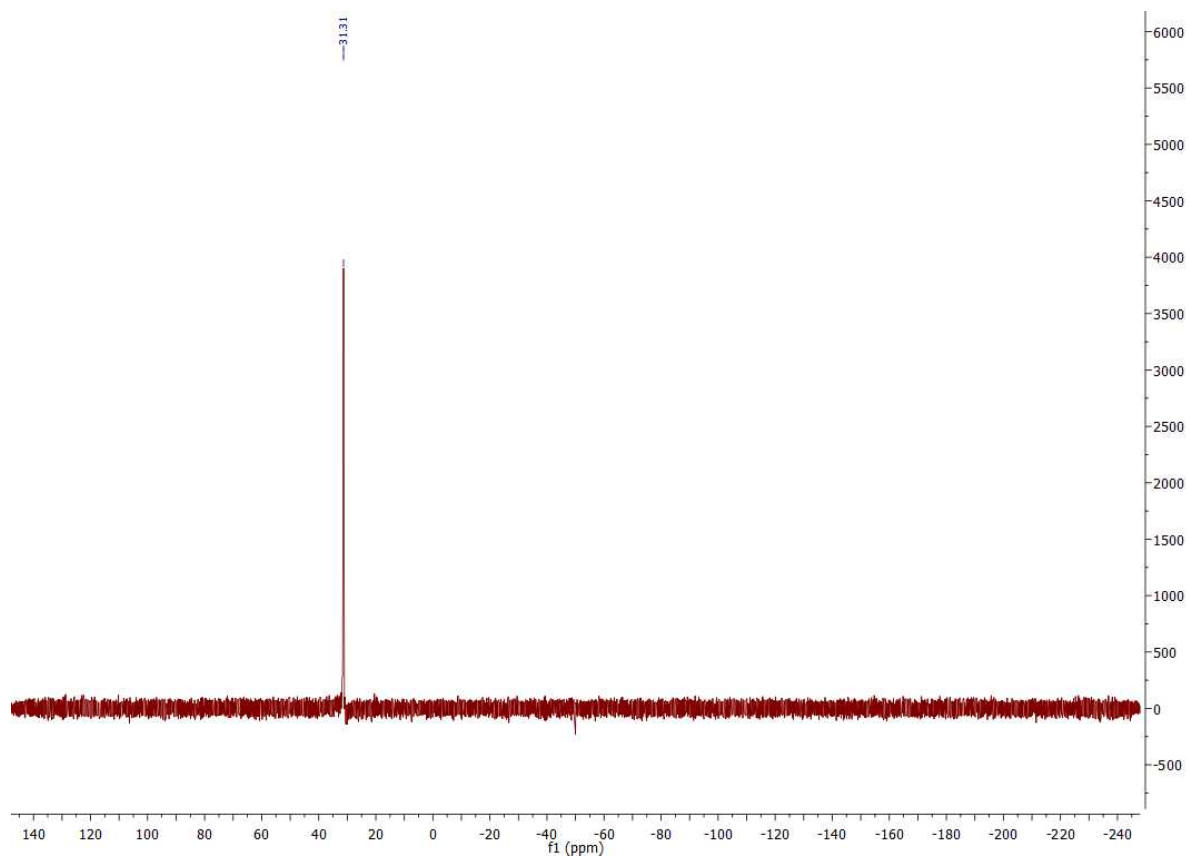


Figure S 24: ^{31}P -NMR of **2b** (162 MHz, C_6D_6).

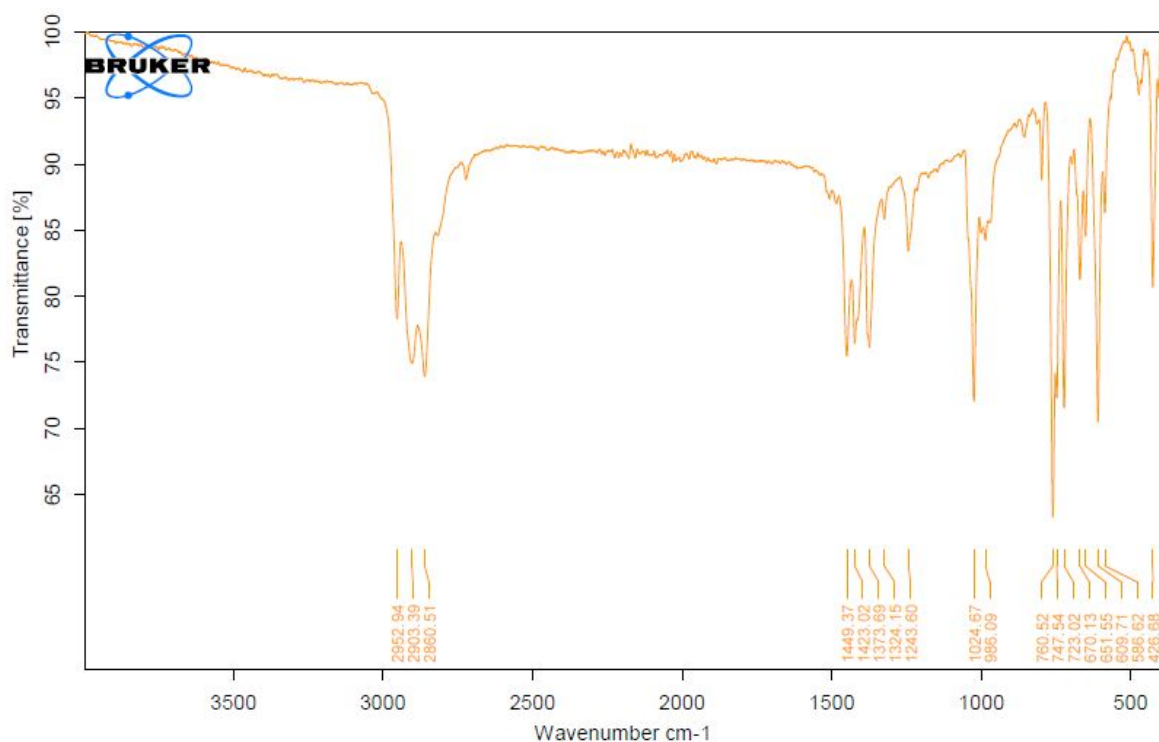


Figure S 25: IR Spectrum of **2b**.

Synthesis Attempt of $[\text{Ni}(\text{GaCp}^*)_3(\text{PEt}_3)]$:

$\text{Ni}(\text{cod})_2$ (200 mg, 0.73 mmol, 1.0 eq.) was added to a Schlenkflask and suspended in 5 mL of hexane. Then GaCp^* (448 mg, 2.15 mmol, 3.0 eq.) was added to the yellow suspension. Triethyl phosphine (86.3 mg, 0.73 mmol, 1.0 eq.) was dissolved in toluene (0.73 mL) to obtain a 1 M solution and added to the reaction mixture. An orange solution was obtained which was stirred for 1h at rt. After removing the solvent an orange solid was obtained, which was washed with 2.5 mL of cold hexane. A yellow to orange powder was obtained. ^1H -NMR indicates that a mixture of different $[\text{Ni}(\text{GaCp}^*)_a(\text{PEt}_3)_{4-a}]$ species was obtained.

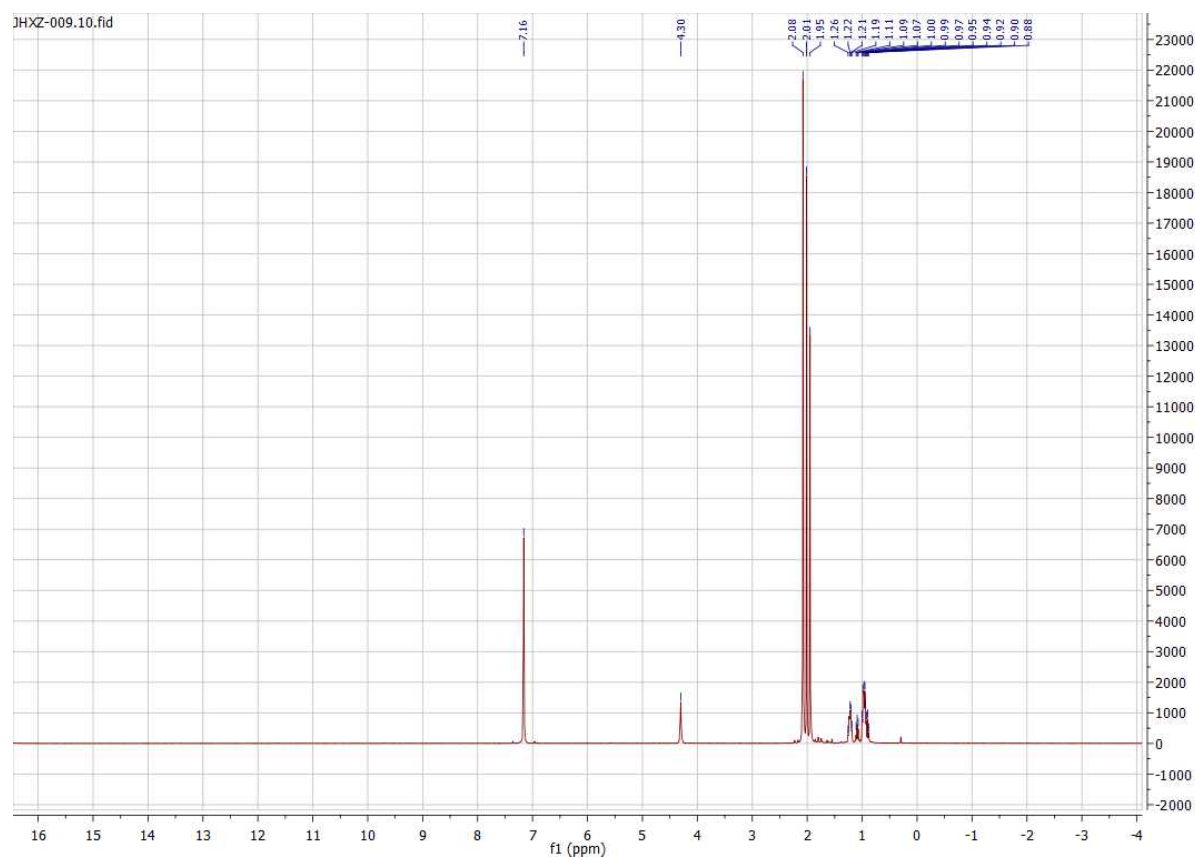


Figure S 24: ^1H -NMR spectrum of the attempt to synthesize **3b**.

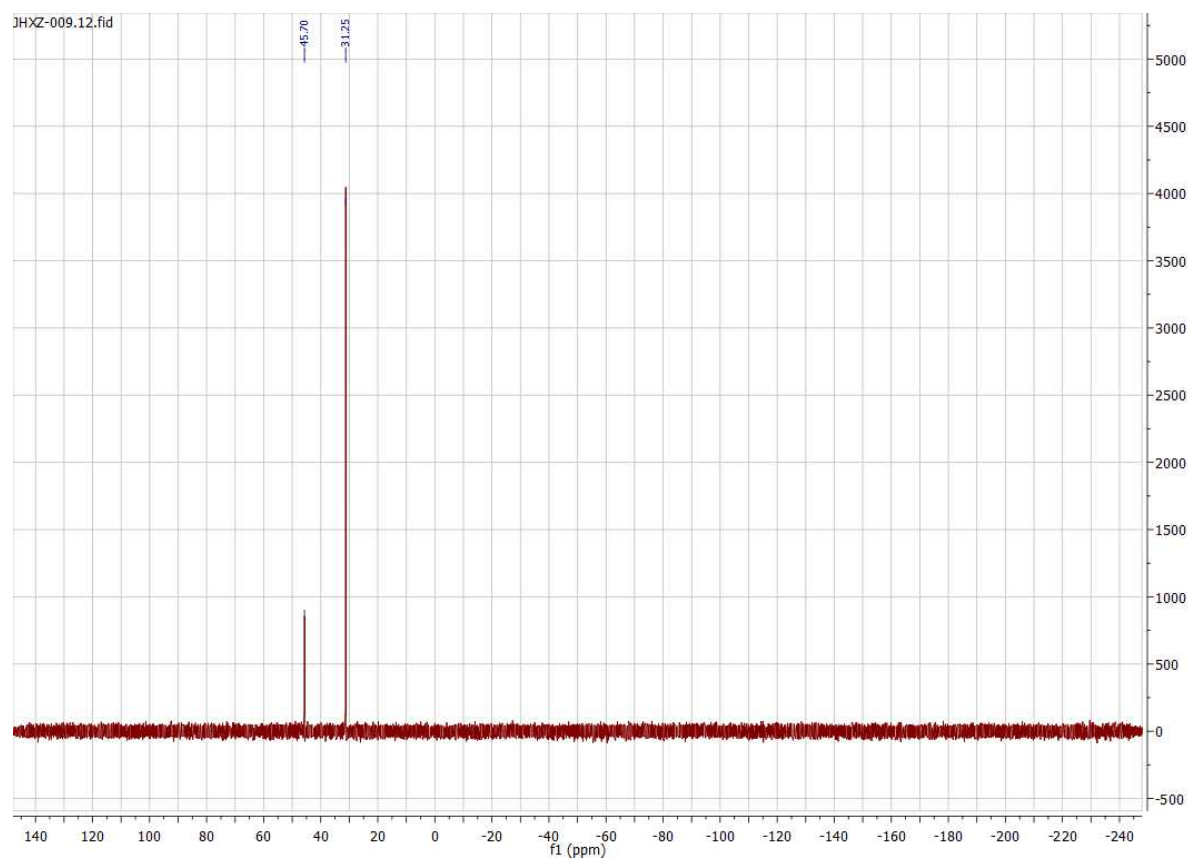


Figure S 25: ^{31}P -NMR spectrum of the attempt to synthesize **3b**.

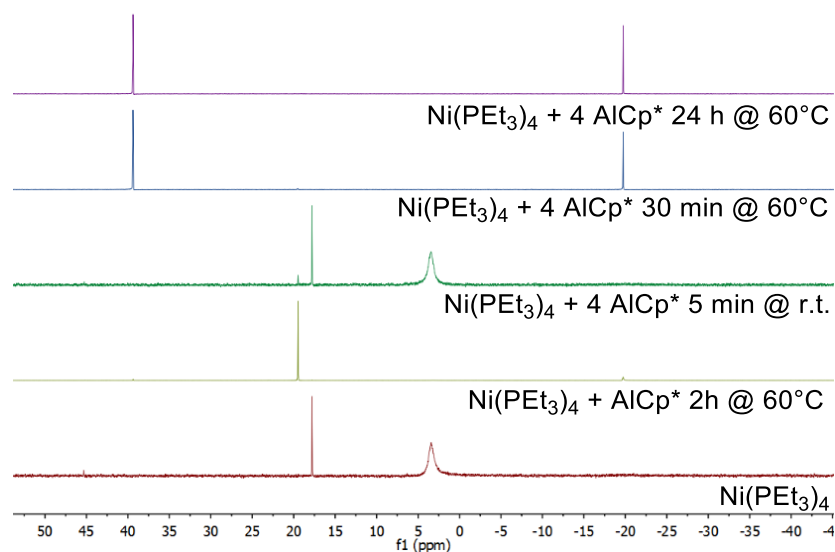


Figure S 26: ^1H -NMR spectrum of the NMR-scale reaction of **5** with 1 or 4 eq. AlCp^* .

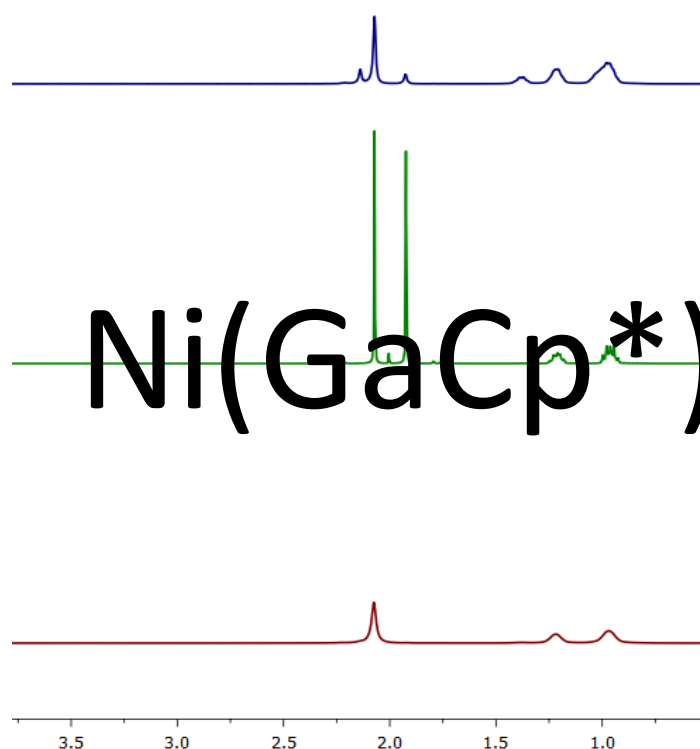


Figure S 27: ^1H -NMR spectrum of the NMR-scale reaction of **2b** with either GaCp^* (no reaction) or PEt_3 (formation of $[\text{Ni}(\text{GaCp}^*)(\text{PEt}_3)_3]$).

VT-UV-Vis Spectra:

1a $\text{Ni}(\text{AlCp}^*)(\text{PEt}_3)_3$:

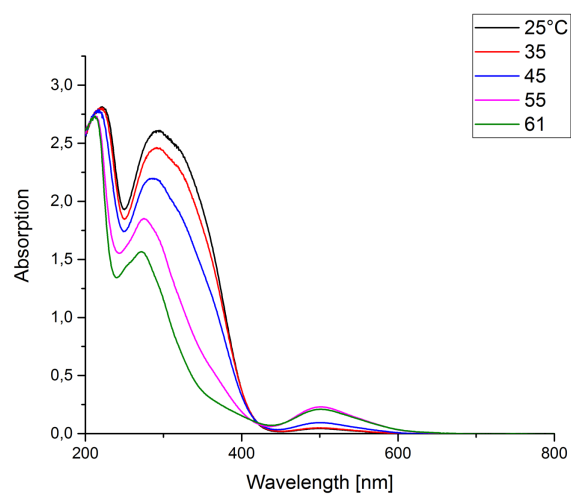


Figure S 28: VT-UV-Vis of **1a** in Hexane.

2a $\text{Ni}(\text{AlCp}^*)_2(\text{PEt}_3)_2$:

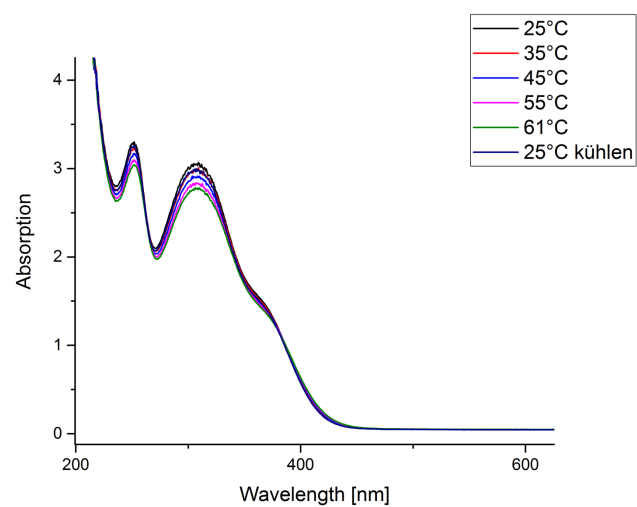


Figure S 29: VT-UV-Vis of **2a** in Hexane.

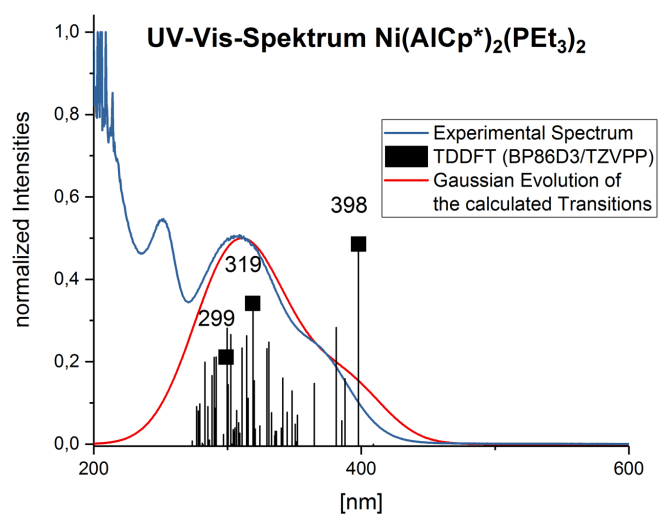


Figure S 30: Comparison of the r.t. UV-Vis of **2a** in Hexane to the TDDFT- calculated absorptions showing nice agreement between theory and experiment.

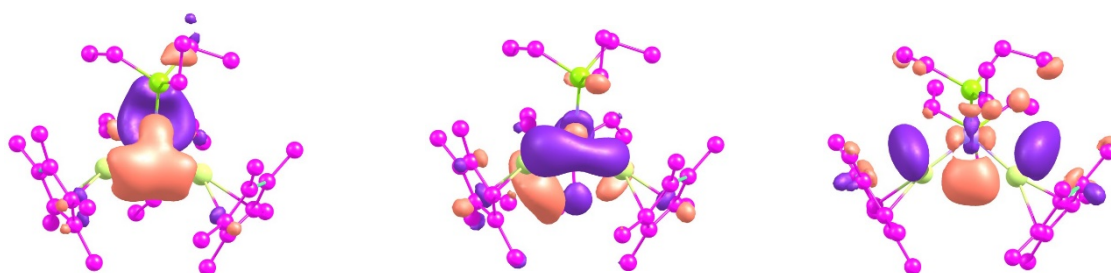


Figure S 31: MO's of **2a** mostly participating in the (calculated) most intense transition at 398 nm. Left: HOMO-1. Middle: LUMO. Right: LUMO+1.

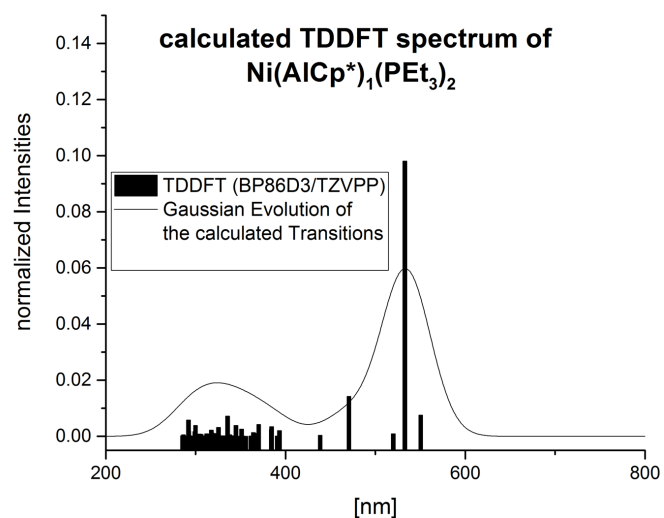


Figure S 32: Calculated TDDFT-spectrum of the potential dissociation product $[\text{Ni}(\text{AlCp}^*)_1(\text{PEt}_3)_2]$

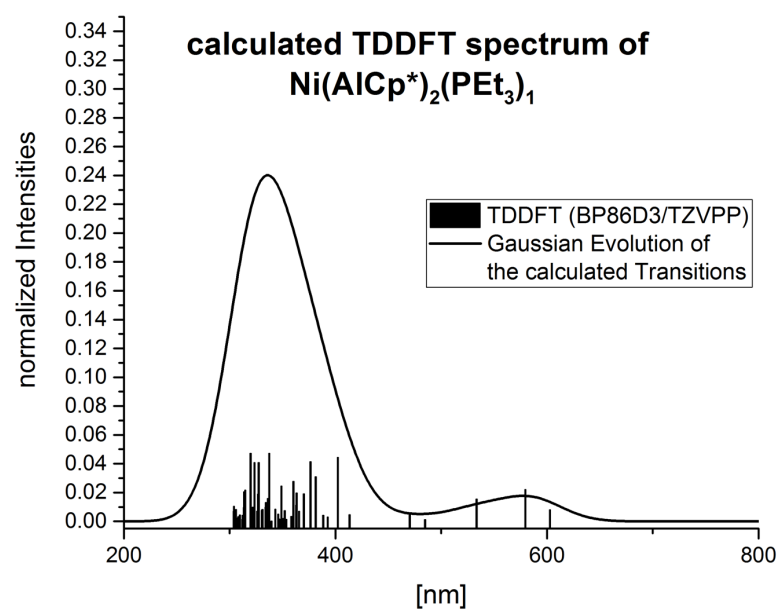


Figure S 33: Calculated TDDFT-spectrum of the potential dissociation product [Ni(AlCp*)₂(PEt₃)₁].

3a $\text{Ni}(\text{AlCp}^*)_3(\text{PEt}_3)_1$:

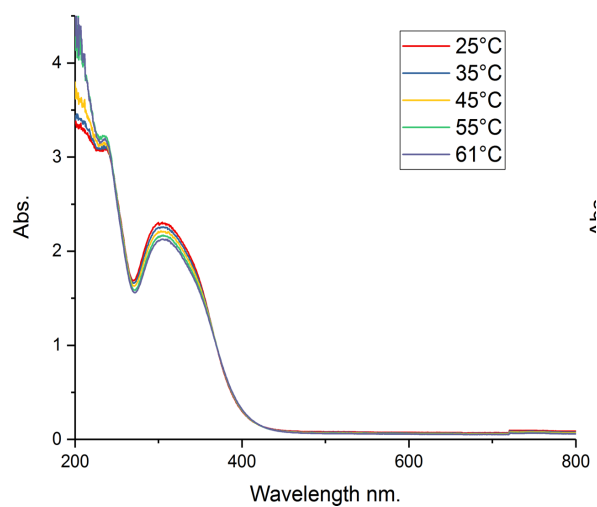


Figure S 31: VT-UV-Vis of **3a** in Hexane.

4a $\text{Ni}(\text{AlCp}^*)_4$:

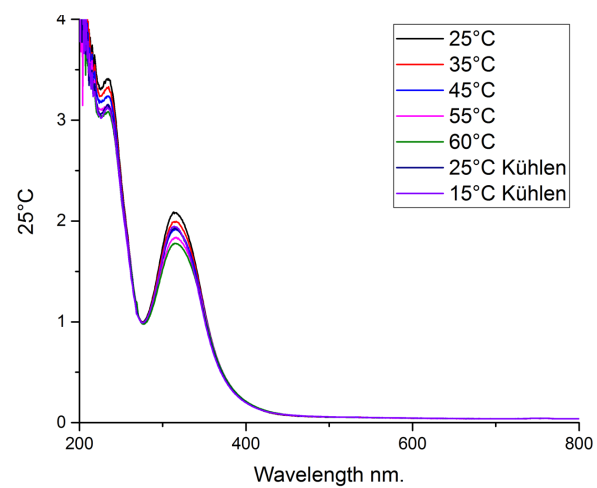


Figure S 32: VT-UV-Vis of **4a** in Hexane.

Table S33: Crystallographic data of compounds **2b** and **3a**.

	2b	3a
Empirical formula	C ₆₄ H ₁₂₀ Ga ₄ Ni ₂ P ₄	C ₃₆ H ₆₀ Al ₃ Ni P
Formula weight	1409.77	663.44
Temperature (K)	100	100
λ (Å)	0.71073	0.71073
Crystal size/mm ³	0.084*0.092*0.223	0.124*0.070*0.059
Crystal system	monoclinic	orthorhombic
Space group	P 1 2/n 1	Pna2 ₁
a/Å	14.567(8)	17.5103(7)
b/Å	16.615(10)	11.9425(5)
c/Å	29.858(19)	18.4956(8)
α /°	90	90
β /°	90.19(2)	90
γ /°	90	90
Volume/Å ³	7227.(8)	3867.7(3)
Z	4	4
ρ g/cm ³	1.296	1.139
μ /mm ⁻¹	2.103	0.633
F(000)	2976	1432
Θ range [°] of data collection	2.30 – 25.03	25.03
Index ranges	-17 ≤ h ≤ 17 -19 ≤ k ≤ 19 -35 ≤ l ≤ 35	-20 ≤ h ≤ 20 -14 ≤ k ≤ 14 -22 ≤ l ≤ 22
Reflections collected/unique	170654/12776	59118/6841
R _{int}	0.0598	0.0657
Reflections observed [$I \geq 2\sigma$]	11081	6017
Data/restraints/parameters	12776/532/912	6841/1/389
Goodness-of-fit on F ²	1.036	1.040
Final R indexes [$I \geq 2\sigma$]	0.0291	0.0316
Final R indexes [all data]	0.0402	0.0407
wR ₂ [all data]	0.0597	0.0656
$\Delta F_{\max}, \Delta F_{\min}$ e Å ⁻³	0.836/-0.639	0.048/-0.301

Theoretical Results:

Coordinates of BP86-D3/TZVPP optimized molecules

1a Ni(AlCp*)₁(PEt₃)₃:

C	-4.428981000000	-0.470774000000	1.139596000000
C	-4.390402000000	0.855300000000	0.605735000000
C	-4.351476000000	0.756971000000	-0.822273000000
C	-4.367982000000	-0.631044000000	-1.169932000000
C	-4.411886000000	-1.388896000000	0.043187000000
Al	-2.423988000000	-0.202492000000	0.010496000000
Ni	-0.210855000000	-0.155433000000	0.066245000000
P	0.295792000000	-2.239677000000	0.164201000000
C	-0.531923000000	-3.321822000000	-1.117072000000
C	-0.116373000000	-4.788995000000	-1.238951000000
P	0.293527000000	0.714939000000	-1.841402000000
C	-0.745140000000	0.102136000000	-3.276232000000
C	-0.212776000000	0.124029000000	-4.710425000000
P	0.078861000000	1.056859000000	1.821950000000
C	-0.454519000000	2.842794000000	1.688128000000
C	-0.370742000000	3.735891000000	2.925777000000
C	0.107787000000	2.573248000000	-1.953996000000
C	-0.117469000000	3.264657000000	-3.300771000000
C	2.047648000000	0.403770000000	-2.423240000000
C	2.728577000000	1.340860000000	-3.423813000000
C	1.813978000000	1.278352000000	2.474906000000
C	2.712331000000	1.957006000000	1.439571000000
C	-0.881842000000	0.522077000000	3.347355000000
C	-0.252295000000	0.680408000000	4.732511000000
C	-0.132875000000	-3.200453000000	1.706281000000

C	0.685770000000	-2.795899000000	2.933157000000
C	2.079545000000	-2.734278000000	-0.113703000000
C	3.082586000000	-1.803837000000	0.569543000000
H	0.991168000000	2.986700000000	-1.441461000000
H	-0.742016000000	2.781226000000	-1.288501000000
H	2.046026000000	-0.634269000000	-2.793234000000
H	2.636198000000	0.374770000000	-1.495619000000
H	-1.687575000000	0.667256000000	-3.195342000000
H	-1.007927000000	-0.926274000000	-2.990610000000
H	1.822064000000	1.839153000000	3.420871000000
H	2.188019000000	0.267940000000	2.693889000000
H	-1.834655000000	1.072729000000	3.287217000000
H	-1.140678000000	-0.529410000000	3.167306000000
H	-0.033410000000	-4.282051000000	1.527050000000
H	-1.200992000000	-2.991771000000	1.873251000000
H	2.240952000000	-3.781497000000	0.186304000000
H	2.222928000000	-2.690002000000	-1.205128000000
H	-1.608438000000	-3.232400000000	-0.904605000000
H	-0.376420000000	-2.798193000000	-2.072460000000
H	0.135853000000	3.266413000000	0.863257000000
H	-1.487908000000	2.792253000000	1.313449000000
H	0.652114000000	3.787956000000	3.324240000000
H	-0.682829000000	4.764334000000	2.690811000000
H	-1.023741000000	3.373200000000	3.730858000000
H	2.441279000000	3.013266000000	1.304596000000
H	3.769531000000	1.919953000000	1.736664000000
H	2.611890000000	1.465030000000	0.461248000000
H	-0.002484000000	1.723902000000	4.962116000000

H	-0.940955000000	0.324124000000	5.512957000000
H	0.671941000000	0.093522000000	4.820371000000
H	4.109212000000	-1.998243000000	0.227428000000
H	2.831931000000	-0.757071000000	0.352651000000
H	3.065966000000	-1.917594000000	1.660659000000
H	0.241181000000	-3.186026000000	3.859528000000
H	1.711639000000	-3.182098000000	2.871995000000
H	0.747738000000	-1.703018000000	3.021555000000
H	-0.704895000000	-5.297882000000	-2.016531000000
H	0.942633000000	-4.890018000000	-1.511212000000
H	-0.271935000000	-5.339989000000	-0.301605000000
H	3.767407000000	1.024230000000	-3.601472000000
H	2.218710000000	1.361903000000	-4.393818000000
H	2.764651000000	2.369739000000	-3.041486000000
H	0.715112000000	-0.456715000000	-4.800549000000
H	-0.944574000000	-0.325625000000	-5.398314000000
H	-0.006483000000	1.140341000000	-5.065584000000
H	-1.020895000000	2.884301000000	-3.796233000000
H	-0.258097000000	4.346688000000	-3.158161000000
H	0.724255000000	3.128989000000	-3.989545000000
C	-4.298503000000	1.910448000000	-1.777577000000
C	-4.348436000000	-1.198559000000	-2.556601000000
C	-4.407123000000	2.126444000000	1.398668000000
C	-4.452788000000	-2.882763000000	0.152414000000
C	-4.486751000000	-0.842558000000	2.589659000000
H	-3.890392000000	-3.241691000000	1.025644000000
H	-5.486109000000	-3.250205000000	0.255922000000
H	-4.024454000000	-3.363828000000	-0.736808000000

H	-3.933382000000	-1.770153000000	2.791104000000
H	-4.055062000000	-0.058981000000	3.225579000000
H	-5.524785000000	-1.001772000000	2.922153000000
H	-3.917447000000	2.002698000000	2.374257000000
H	-3.889139000000	2.938469000000	0.870868000000
H	-5.436819000000	2.467195000000	1.590968000000
H	-3.715654000000	2.747193000000	-1.368583000000
H	-3.834393000000	1.623422000000	-2.730602000000
H	-5.305668000000	2.292772000000	-2.006981000000
H	-3.778208000000	-2.136577000000	-2.602143000000
H	-5.366753000000	-1.414567000000	-2.916369000000
H	-3.888997000000	-0.503152000000	-3.270682000000

2a Ni(AlCp*)₂(PEt₃)₂:

C	-3.273026000000	5.978203000000	5.442545000000
C	-3.969620000000	5.058315000000	4.597761000000
C	-3.622620000000	5.351756000000	3.242210000000
C	-2.714031000000	6.457983000000	3.245391000000
C	-2.497393000000	6.844882000000	4.606719000000
Al	-1.684780000000	4.719423000000	4.343829000000
Ni	-0.039112000000	3.250455000000	4.330591000000
P	-0.043995000000	2.174200000000	6.173373000000
C	-1.096709000000	0.636913000000	6.251614000000
C	-4.897924000000	3.971233000000	5.044680000000
C	-1.626934000000	7.967501000000	5.081215000000
C	-4.129625000000	4.620479000000	2.036599000000
C	-2.100103000000	7.103197000000	2.040455000000
C	-3.350798000000	6.045313000000	6.937400000000

Al	1.658893000000	4.649939000000	4.312728000000
C	3.325500000000	5.427715000000	2.902729000000
C	3.953112000000	4.652258000000	3.926048000000
C	3.695880000000	5.285359000000	5.181922000000
C	2.913148000000	6.460523000000	4.934125000000
C	2.686892000000	6.548033000000	3.522906000000
C	4.723219000000	3.385136000000	3.714906000000
C	1.935445000000	7.629509000000	2.809749000000
C	4.164746000000	4.808915000000	6.523112000000
C	2.436757000000	7.434518000000	5.968592000000
C	3.344278000000	5.129464000000	1.434933000000
P	-0.093164000000	2.383530000000	2.378091000000
C	1.412034000000	1.385803000000	1.886843000000
C	-1.518612000000	1.200903000000	2.105577000000
C	-0.280108000000	3.623701000000	0.988439000000
C	1.575785000000	1.499076000000	6.798263000000
C	-0.629731000000	3.106783000000	7.678007000000
C	-2.059456000000	0.942342000000	0.697183000000
H	-2.315822000000	1.615925000000	2.738702000000
H	-1.217257000000	0.260481000000	2.593952000000
H	4.211172000000	5.595427000000	0.940098000000
H	2.441901000000	5.503481000000	0.933319000000
H	3.403536000000	4.049409000000	1.244081000000
H	5.140309000000	5.246440000000	6.787931000000
H	4.279355000000	3.716887000000	6.544744000000
H	3.457881000000	5.081841000000	7.318317000000
H	5.777314000000	3.590622000000	3.470280000000
H	4.304752000000	2.791249000000	2.890755000000

H	4.711271000000	2.752258000000	4.611428000000
H	3.183288000000	8.223266000000	6.152611000000
H	2.240984000000	6.939006000000	6.929131000000
H	1.506210000000	7.928220000000	5.659382000000
C	0.222822000000	3.307545000000	-0.420724000000
H	0.225914000000	4.518677000000	1.378641000000
H	-1.351407000000	3.877859000000	0.978007000000
H	2.615267000000	8.406110000000	2.425225000000
H	1.218337000000	8.125567000000	3.476548000000
H	1.372131000000	7.234622000000	1.952759000000
C	1.323950000000	0.294293000000	0.817523000000
H	1.754111000000	0.948554000000	2.834757000000
H	2.174015000000	2.136986000000	1.624801000000
H	1.406171000000	0.831380000000	7.657187000000
H	2.137701000000	2.372917000000	7.163920000000
C	2.370557000000	0.790216000000	5.702943000000
H	-4.110052000000	6.772015000000	7.267401000000
H	-2.392223000000	6.349517000000	7.379248000000
H	-3.619628000000	5.073242000000	7.371510000000
H	-5.131119000000	4.972594000000	1.743085000000
H	-4.204320000000	3.539320000000	2.219491000000
H	-3.468995000000	4.763631000000	1.171598000000
H	-5.945066000000	4.313182000000	5.047303000000
H	-4.661727000000	3.629336000000	6.060700000000
H	-4.841456000000	3.095659000000	4.383838000000
H	-2.712909000000	7.943117000000	1.676982000000
H	-1.992980000000	6.391162000000	1.211566000000
H	-1.099814000000	7.497963000000	2.261904000000

C	-0.646311000000	2.386334000000	9.026395000000
H	-1.633503000000	3.470502000000	7.413052000000
H	0.005378000000	4.005234000000	7.710921000000
H	-2.207578000000	8.890025000000	5.239552000000
H	-0.840447000000	8.198055000000	4.350789000000
H	-1.133325000000	7.722536000000	6.031832000000
H	-0.969608000000	0.132243000000	7.222571000000
H	-0.692142000000	-0.037157000000	5.481925000000
C	-2.570410000000	0.930094000000	5.970795000000
H	-2.925396000000	0.264482000000	0.734870000000
H	-2.398530000000	1.874673000000	0.225737000000
H	-1.311736000000	0.486842000000	0.037617000000
H	2.294972000000	-0.210673000000	0.703381000000
H	0.590234000000	-0.474689000000	1.094101000000
H	1.039970000000	0.690035000000	-0.164458000000
H	0.083723000000	4.175839000000	-1.082151000000
H	1.295498000000	3.071854000000	-0.417923000000
H	-0.305425000000	2.460128000000	-0.873437000000
H	3.348024000000	0.445774000000	6.070502000000
H	1.831922000000	-0.087354000000	5.317632000000
H	2.531800000000	1.476876000000	4.859735000000
H	-3.155978000000	0.005843000000	5.866103000000
H	-3.021437000000	1.520494000000	6.781038000000
H	-2.669193000000	1.517355000000	5.046845000000
H	-1.028350000000	3.046398000000	9.818942000000
H	-1.291451000000	1.497059000000	9.003592000000
H	0.357947000000	2.059959000000	9.327870000000

3a Ni(AlCp*)₃(PEt₃)₁:

(two small negative frequencies using def2-TZVPP, -6.1 and -5.4 cm⁻¹):

C	-2.393646000000	3.506958000000	-2.347128000000
C	-3.231145000000	2.572655000000	-3.041472000000
C	-3.005231000000	2.736341000000	-4.446542000000
C	-2.032485000000	3.769601000000	-4.621105000000
C	-1.653986000000	4.244186000000	-3.326691000000
Al	-1.034288000000	2.049122000000	-3.471794000000
Ni	0.788874000000	0.909828000000	-3.898822000000
C	-4.196528000000	1.611016000000	-2.418125000000
C	-0.633956000000	5.307830000000	-3.064631000000
C	-3.667629000000	1.947209000000	-5.534500000000
C	-1.443557000000	4.246163000000	-5.913183000000
C	-2.331448000000	3.711829000000	-0.863964000000
Al	2.357141000000	2.437471000000	-3.798141000000
C	4.287030000000	3.127516000000	-4.850430000000
C	4.645527000000	2.245860000000	-3.783555000000
C	4.229614000000	2.845991000000	-2.554428000000
C	3.613976000000	4.102792000000	-2.857460000000
C	3.649562000000	4.276875000000	-4.280360000000
C	5.284425000000	0.896541000000	-3.904170000000
C	3.140494000000	5.462056000000	-5.043034000000
C	4.390450000000	2.230634000000	-1.199415000000
C	3.067148000000	5.074704000000	-1.856428000000
C	4.517878000000	2.891334000000	-6.311917000000
P	0.751125000000	-0.244259000000	-5.676859000000
C	2.416924000000	-0.922362000000	-6.183235000000
C	-0.356017000000	-1.746979000000	-5.588463000000

C	0.149549000000	0.685614000000	-7.181784000000
C	-0.939624000000	-2.361591000000	-6.862767000000
H	-1.165629000000	-1.424070000000	-4.918832000000
H	0.218660000000	-2.490567000000	-5.013894000000
H	5.473416000000	3.325657000000	-6.645860000000
H	3.723116000000	3.340349000000	-6.922851000000
H	4.545818000000	1.818706000000	-6.545647000000
H	5.429175000000	2.304020000000	-0.841054000000
H	4.120567000000	1.163724000000	-1.218053000000
H	3.746957000000	2.718870000000	-0.456997000000
H	6.341334000000	0.921170000000	-3.596088000000
H	5.248034000000	0.525377000000	-4.935871000000
H	4.769456000000	0.158432000000	-3.271068000000
H	3.864673000000	5.707221000000	-1.435779000000
H	2.579603000000	4.560604000000	-1.016627000000
H	2.323562000000	5.743277000000	-2.307770000000
C	0.562611000000	0.242302000000	-8.587194000000
H	0.486993000000	1.714831000000	-6.995079000000
H	-0.946793000000	0.714442000000	-7.078699000000
H	3.945411000000	6.186521000000	-5.244715000000
H	2.356170000000	5.993603000000	-4.488349000000
H	2.716350000000	5.168108000000	-6.013155000000
C	2.515416000000	-2.176144000000	-7.055282000000
H	2.923791000000	-1.088759000000	-5.222271000000
H	2.941369000000	-0.071813000000	-6.646911000000
H	-2.989321000000	4.536142000000	-0.546633000000
H	-1.313718000000	3.958279000000	-0.531310000000
H	-2.645604000000	2.813117000000	-0.318777000000

H	-4.628062000000	2.396686000000	-5.832304000000
H	-3.873276000000	0.915966000000	-5.216787000000
H	-3.037951000000	1.894469000000	-6.432551000000
H	-5.217076000000	2.024854000000	-2.392910000000
H	-3.917377000000	1.370839000000	-1.383810000000
H	-4.242543000000	0.664804000000	-2.975036000000
H	-1.830645000000	5.238391000000	-6.192506000000
H	-1.669809000000	3.557063000000	-6.736244000000
H	-0.348020000000	4.323181000000	-5.842460000000
H	-1.036690000000	6.313822000000	-3.261106000000
H	0.248750000000	5.172286000000	-3.707629000000
H	-0.288047000000	5.285549000000	-2.023637000000
H	-1.603464000000	-3.203333000000	-6.614924000000
H	-1.539928000000	-1.628648000000	-7.418406000000
H	-0.164294000000	-2.740517000000	-7.539030000000
H	3.568348000000	-2.455355000000	-7.210298000000
H	2.020436000000	-3.032248000000	-6.577401000000
H	2.061931000000	-2.036155000000	-8.043612000000
H	0.156393000000	0.930903000000	-9.343136000000
H	1.655165000000	0.246061000000	-8.699707000000
H	0.204599000000	-0.764790000000	-8.831397000000
Al	1.098392000000	-0.229052000000	-2.052105000000
C	-0.082705000000	-0.719644000000	-0.159134000000
H	-1.798593000000	-0.306957000000	1.088087000000
C	-1.206766000000	0.162594000000	0.286578000000
H	-1.890462000000	0.378492000000	-0.547871000000
H	-0.837873000000	1.123832000000	0.666186000000
C	-0.212368000000	-1.830111000000	-1.050139000000

C	-1.491766000000	-2.261820000000	-1.698240000000
H	-2.158156000000	-2.765889000000	-0.981252000000
H	-1.308125000000	-2.957149000000	-2.526551000000
H	-2.036499000000	-1.398465000000	-2.109895000000
C	1.087689000000	-2.390735000000	-1.250424000000
C	1.426099000000	-3.560422000000	-2.123583000000
H	1.442153000000	-4.501154000000	-1.551013000000
H	2.414387000000	-3.443560000000	-2.588906000000
H	0.694925000000	-3.681236000000	-2.933740000000
C	2.023116000000	-1.627459000000	-0.479496000000
C	3.494778000000	-1.890960000000	-0.379415000000
H	3.717325000000	-2.645814000000	0.391368000000
H	3.904617000000	-2.263625000000	-1.328354000000
H	4.051828000000	-0.982383000000	-0.115099000000
C	1.297877000000	-0.592563000000	0.198336000000
C	1.869501000000	0.417888000000	1.145781000000
H	1.764030000000	0.088739000000	2.191529000000
H	2.938126000000	0.584232000000	0.961290000000
H	1.364892000000	1.389665000000	1.055479000000

4a Ni(AlCp*)₄:

Al	7.248437000000	13.523955000000	17.461928000000
Ni	6.138085000000	12.096590000000	18.681875000000
C	8.618418000000	15.305868000000	17.081616000000
C	8.462021000000	14.575426000000	15.854560000000
C	7.079939000000	14.640755000000	15.477254000000
C	6.387735000000	15.404478000000	16.467045000000
C	7.334085000000	15.815265000000	17.455901000000
C	9.909278000000	15.530024000000	17.809046000000

C	9.561290000000	13.911068000000	15.082076000000
C	6.456272000000	14.007721000000	14.270819000000
C	4.912604000000	15.660830000000	16.529107000000
C	6.990877000000	16.585067000000	18.694069000000
H	10.421079000000	16.435317000000	17.446078000000
H	10.601023000000	14.688214000000	17.673752000000
H	9.749649000000	15.651233000000	18.888370000000
H	10.024683000000	14.605951000000	14.363912000000
H	9.190630000000	13.049145000000	14.511326000000
H	10.358247000000	13.548225000000	15.745045000000
H	7.091074000000	13.209909000000	13.865482000000
H	6.296132000000	14.742264000000	13.466190000000
H	5.481816000000	13.561101000000	14.514032000000
H	4.700940000000	16.720822000000	16.731385000000
H	4.442496000000	15.065469000000	17.330131000000
H	4.419915000000	15.393352000000	15.586469000000
H	7.877380000000	16.773763000000	19.311544000000
H	6.266093000000	16.031057000000	19.313777000000
H	6.540834000000	17.558565000000	18.447308000000
Al	4.956275000000	10.841992000000	17.347459000000
C	3.224150000000	9.559928000000	16.582034000000
C	3.865756000000	10.175050000000	15.454433000000
C	5.210038000000	9.686223000000	15.391976000000
C	3.217432000000	11.130112000000	14.498649000000
H	2.664162000000	10.595867000000	13.710159000000
H	3.959099000000	11.769328000000	14.002295000000
H	2.503356000000	11.790845000000	15.008884000000
C	5.401221000000	8.780090000000	16.482011000000

C	4.175328000000	8.695932000000	17.214148000000
C	1.792653000000	9.754552000000	16.979265000000
H	1.126486000000	9.086062000000	16.411144000000
H	1.455381000000	10.783388000000	16.792767000000
H	1.633999000000	9.543733000000	18.044746000000
C	6.680558000000	8.082728000000	16.825249000000
H	6.776109000000	7.122924000000	16.292974000000
H	6.738527000000	7.874606000000	17.901532000000
H	7.551589000000	8.699085000000	16.564619000000
C	3.963279000000	7.882346000000	18.454238000000
H	3.064671000000	8.202443000000	18.996289000000
H	4.814460000000	7.981896000000	19.144183000000
H	3.847337000000	6.812723000000	18.220985000000
C	6.263055000000	10.072956000000	14.398834000000
H	5.949277000000	10.934898000000	13.797967000000
H	6.482759000000	9.246995000000	13.705180000000
H	7.204271000000	10.345637000000	14.899487000000
Al	4.805039000000	13.199237000000	20.007263000000
C	3.262963000000	14.784992000000	20.622557000000
C	4.029156000000	14.414945000000	21.778204000000
C	3.789896000000	13.026626000000	22.039880000000
C	4.895828000000	15.331178000000	22.587799000000
H	4.325603000000	15.813195000000	23.397645000000
H	5.731601000000	14.790627000000	23.051764000000
H	5.324895000000	16.130949000000	21.969434000000
C	2.887599000000	12.538508000000	21.042534000000
C	2.560641000000	13.623193000000	20.169233000000
C	3.176841000000	16.160796000000	20.035593000000

H	2.389523000000	16.753358000000	20.527739000000
H	4.119609000000	16.711527000000	20.151508000000
H	2.944819000000	16.131873000000	18.963485000000
C	2.409877000000	11.128403000000	20.882754000000
H	1.374290000000	11.007677000000	21.237380000000
H	2.440771000000	10.822527000000	19.826869000000
H	3.040524000000	10.426647000000	21.442436000000
C	1.679975000000	13.515592000000	18.962462000000
H	1.758053000000	14.405958000000	18.326361000000
H	1.958988000000	12.646105000000	18.347547000000
H	0.622124000000	13.397572000000	19.243270000000
C	4.395718000000	12.217609000000	23.144870000000
H	5.339205000000	12.659448000000	23.491084000000
H	3.723177000000	12.152778000000	24.014364000000
H	4.613928000000	11.192423000000	22.816111000000
Al	7.452665000000	10.859270000000	19.906584000000
C	8.644719000000	9.096367000000	20.741740000000
C	8.189689000000	9.894348000000	21.844514000000
C	8.791692000000	11.188089000000	21.731045000000
C	7.277100000000	9.421358000000	22.934752000000
H	7.828906000000	8.852578000000	23.699803000000
H	6.784575000000	10.260573000000	23.441063000000
H	6.488245000000	8.762660000000	22.545506000000
C	9.611745000000	11.192227000000	20.558756000000
C	9.526410000000	9.900108000000	19.949470000000
C	8.293029000000	7.658437000000	20.509794000000
H	8.906550000000	6.991724000000	21.136251000000
H	7.240748000000	7.452269000000	20.751308000000

H	8.456464000000	7.366018000000	19.464924000000
C	10.383783000000	12.361160000000	20.031611000000
H	11.425704000000	12.355704000000	20.389070000000
H	10.407508000000	12.357829000000	18.933186000000
H	9.928238000000	13.310387000000	20.342860000000
C	10.220065000000	9.491790000000	18.685776000000
H	9.758047000000	8.600310000000	18.243323000000
H	10.179547000000	10.291847000000	17.932525000000
H	11.281332000000	9.260106000000	18.865803000000
C	8.568119000000	12.364671000000	22.632020000000
H	7.745468000000	12.178155000000	23.333368000000
H	9.465227000000	12.593214000000	23.227257000000
H	8.310393000000	13.265838000000	22.055467000000

1b Ni(GaCp*)₁(PEt₃)₃:

C	-4.553223000000	-0.394855000000	1.094497000000
C	-4.387324000000	0.938282000000	0.600921000000
C	-4.321681000000	0.877958000000	-0.827622000000
C	-4.448258000000	-0.492817000000	-1.218185000000
C	-4.589024000000	-1.280225000000	-0.029867000000
Ga	-2.372740000000	-0.305903000000	0.035468000000
Ni	-0.100013000000	-0.196396000000	0.082538000000
P	0.457682000000	-2.273373000000	0.184935000000
C	-0.372224000000	-3.375565000000	-1.075460000000
C	0.045436000000	-4.844188000000	-1.172966000000
P	0.286855000000	0.682531000000	-1.851345000000
C	-0.769470000000	0.005040000000	-3.240367000000
C	-0.282264000000	0.034522000000	-4.690352000000
P	0.104082000000	1.044052000000	1.835413000000

C	-0.467866000000	2.812865000000	1.669075000000
C	-0.435389000000	3.721445000000	2.897969000000
C	0.006193000000	2.527154000000	-1.975973000000
C	-0.277647000000	3.195108000000	-3.323665000000
C	2.037048000000	0.439602000000	-2.464445000000
C	2.648669000000	1.392772000000	-3.494357000000
C	1.828219000000	1.296689000000	2.495650000000
C	2.720687000000	1.986380000000	1.461687000000
C	-0.871634000000	0.499294000000	3.345936000000
C	-0.274693000000	0.701891000000	4.739902000000
C	0.089499000000	-3.236650000000	1.739397000000
C	0.879256000000	-2.761867000000	2.959831000000
C	2.247237000000	-2.704532000000	-0.130029000000
C	3.231976000000	-1.731107000000	0.519435000000
H	0.875597000000	2.989429000000	-1.481462000000
H	-0.841434000000	2.698896000000	-1.297441000000
H	2.073894000000	-0.602583000000	-2.820339000000
H	2.647895000000	0.452020000000	-1.550791000000
H	-1.732928000000	0.528820000000	-3.135851000000
H	-0.978679000000	-1.030800000000	-2.938783000000
H	1.819686000000	1.862877000000	3.438321000000
H	2.218916000000	0.294639000000	2.723289000000
H	-1.841508000000	1.015092000000	3.256539000000
H	-1.090926000000	-0.563619000000	3.181057000000
H	0.258076000000	-4.311998000000	1.575504000000
H	-0.989907000000	-3.095414000000	1.904708000000
H	2.450108000000	-3.740991000000	0.181735000000
H	2.366185000000	-2.672001000000	-1.224676000000

H	-1.449731000000	-3.283726000000	-0.867225000000
H	-0.214606000000	-2.868245000000	-2.039449000000
H	0.131114000000	3.241209000000	0.852912000000
H	-1.490806000000	2.733433000000	1.271984000000
H	0.575615000000	3.799770000000	3.321615000000
H	-0.763360000000	4.739860000000	2.642563000000
H	-1.101642000000	3.353541000000	3.689439000000
H	2.431716000000	3.036841000000	1.320147000000
H	3.776071000000	1.969438000000	1.766607000000
H	2.634869000000	1.487341000000	0.485729000000
H	-0.057836000000	1.756013000000	4.953157000000
H	-0.969355000000	0.342044000000	5.513106000000
H	0.662869000000	0.141843000000	4.857167000000
H	4.261766000000	-1.918383000000	0.182979000000
H	2.962034000000	-0.697844000000	0.265711000000
H	3.217503000000	-1.806556000000	1.613862000000
H	0.467574000000	-3.177116000000	3.890326000000
H	1.931419000000	-3.069424000000	2.898744000000
H	0.857281000000	-1.666689000000	3.038226000000
H	-0.525725000000	-5.359650000000	-1.958908000000
H	1.110397000000	-4.948226000000	-1.420213000000
H	-0.132758000000	-5.385159000000	-0.234132000000
H	3.696129000000	1.121433000000	-3.693697000000
H	2.113731000000	1.375288000000	-4.450781000000
H	2.645824000000	2.427559000000	-3.126777000000
H	0.665434000000	-0.509059000000	-4.803913000000
H	-1.016032000000	-0.451321000000	-5.350676000000
H	-0.128813000000	1.054861000000	-5.060311000000

H	-1.171923000000	2.767922000000	-3.796654000000
H	-0.467065000000	4.270180000000	-3.186462000000
H	0.555961000000	3.092893000000	-4.027904000000
C	-4.163157000000	2.049655000000	-1.748194000000
C	-4.470022000000	-1.017849000000	-2.621264000000
C	-4.342395000000	2.182767000000	1.433654000000
C	-4.777721000000	-2.765894000000	0.021082000000
C	-4.697243000000	-0.787788000000	2.533054000000
H	-4.371908000000	-3.194690000000	0.947694000000
H	-5.843665000000	-3.042703000000	-0.024848000000
H	-4.278499000000	-3.266127000000	-0.820527000000
H	-4.315045000000	-1.801421000000	2.716255000000
H	-4.147614000000	-0.105323000000	3.195957000000
H	-5.751320000000	-0.774695000000	2.854909000000
H	-3.861265000000	2.006091000000	2.406210000000
H	-3.786445000000	2.986691000000	0.932144000000
H	-5.353428000000	2.570153000000	1.640302000000
H	-3.545403000000	2.839089000000	-1.297564000000
H	-3.683693000000	1.759645000000	-2.693443000000
H	-5.133898000000	2.503627000000	-2.005423000000
H	-3.995786000000	-2.006780000000	-2.692524000000
H	-5.500055000000	-1.123442000000	-2.998869000000
H	-3.938850000000	-0.350239000000	-3.312706000000

2b Ni(GaCp*)₂(PEt₃)₂:

C	-2.888746000000	6.361832000000	5.577135000000
C	-3.604196000000	5.234005000000	5.062546000000
C	-3.500159000000	5.255894000000	3.635819000000
C	-2.729855000000	6.402028000000	3.265141000000

C	-2.352808000000	7.089153000000	4.464598000000
Ga	-1.252044000000	4.931793000000	4.537863000000
Ni	0.083709000000	3.095531000000	4.407381000000
P	-0.249283000000	1.857937000000	6.121997000000
C	-1.397199000000	0.411160000000	5.894761000000
C	-4.383322000000	4.247969000000	5.876039000000
C	-1.630709000000	8.399250000000	4.534991000000
C	-4.107909000000	4.261761000000	2.694445000000
C	-2.435894000000	6.856396000000	1.868590000000
C	-2.774802000000	6.745338000000	7.021117000000
Ga	2.089836000000	4.150094000000	4.526693000000
C	3.532426000000	5.326608000000	2.937073000000
C	4.309709000000	4.894228000000	4.060304000000
C	3.832198000000	5.590412000000	5.223455000000
C	2.756202000000	6.440702000000	4.811953000000
C	2.577577000000	6.279710000000	3.402661000000
C	5.471890000000	3.949523000000	4.014876000000
C	1.534636000000	6.985488000000	2.594221000000
C	4.407421000000	5.488804000000	6.603503000000
C	1.929894000000	7.339001000000	5.679261000000
C	3.716745000000	4.869708000000	1.522082000000
P	-0.043632000000	2.434353000000	2.370964000000
C	1.432151000000	1.424203000000	1.835412000000
C	-1.516936000000	1.348857000000	2.003112000000
C	-0.156567000000	3.794354000000	1.098964000000
C	1.246420000000	0.999580000000	6.817677000000
C	-0.946902000000	2.671066000000	7.645446000000
C	-2.044097000000	1.211845000000	0.572845000000

H	-2.308192000000	1.757251000000	2.646385000000
H	-1.270511000000	0.364846000000	2.432561000000
H	4.475540000000	5.470558000000	0.995162000000
H	2.785119000000	4.944423000000	0.945843000000
H	4.048496000000	3.822878000000	1.475375000000
H	5.232099000000	6.204978000000	6.749813000000
H	4.810490000000	4.486325000000	6.802274000000
H	3.653273000000	5.698766000000	7.373895000000
H	6.416567000000	4.480037000000	3.811772000000
H	5.349724000000	3.193856000000	3.226684000000
H	5.598812000000	3.415736000000	4.966433000000
H	2.140783000000	8.402014000000	5.481381000000
H	2.118246000000	7.158215000000	6.745100000000
H	0.854137000000	7.183228000000	5.502832000000
C	0.314233000000	3.568533000000	-0.338470000000
H	0.409270000000	4.618937000000	1.553411000000
H	-1.207658000000	4.121617000000	1.126017000000
H	1.675377000000	8.077369000000	2.618288000000
H	0.521951000000	6.778786000000	2.978999000000
H	1.556761000000	6.674739000000	1.542071000000
C	1.314536000000	0.427413000000	0.680219000000
H	1.740379000000	0.898599000000	2.750018000000
H	2.225695000000	2.163877000000	1.645011000000
H	0.942721000000	0.301911000000	7.613402000000
H	1.855790000000	1.789533000000	7.283180000000
C	2.058215000000	0.276645000000	5.742181000000
H	-3.615903000000	7.382514000000	7.339572000000
H	-1.850287000000	7.304068000000	7.219872000000

H	-2.771740000000	5.862230000000	7.674935000000
H	-5.118318000000	4.564257000000	2.375013000000
H	-4.198266000000	3.269866000000	3.157993000000
H	-3.504076000000	4.143601000000	1.783921000000
H	-5.405172000000	4.610691000000	6.073792000000
H	-3.915142000000	4.062342000000	6.852968000000
H	-4.474226000000	3.281399000000	5.365314000000
H	-3.196217000000	7.569281000000	1.509924000000
H	-2.423926000000	6.016121000000	1.161643000000
H	-1.461714000000	7.358767000000	1.797662000000
C	-1.235986000000	1.800320000000	8.868475000000
H	-1.857640000000	3.184536000000	7.302802000000
H	-0.232589000000	3.473566000000	7.884339000000
H	-2.333672000000	9.244437000000	4.453054000000
H	-0.897520000000	8.509457000000	3.725023000000
H	-1.093216000000	8.518393000000	5.484932000000
H	-1.380019000000	-0.238223000000	6.784342000000
H	-0.977319000000	-0.170501000000	5.061207000000
C	-2.821652000000	0.855737000000	5.565280000000
H	-2.942231000000	0.576956000000	0.554616000000
H	-2.330437000000	2.188897000000	0.161291000000
H	-1.307863000000	0.765511000000	-0.105462000000
H	2.266788000000	-0.103974000000	0.535187000000
H	0.547935000000	-0.331770000000	0.885378000000
H	1.059000000000	0.913790000000	-0.268275000000
H	0.222103000000	4.497233000000	-0.921036000000
H	1.370865000000	3.270616000000	-0.368594000000
H	-0.266614000000	2.795286000000	-0.854681000000

H	2.955614000000	-0.194757000000	6.167149000000
H	1.468195000000	-0.511334000000	5.253086000000
H	2.372805000000	0.988757000000	4.966150000000
H	-3.447862000000	0.011297000000	5.245825000000
H	-3.305216000000	1.321131000000	6.434554000000
H	-2.808345000000	1.602971000000	4.759086000000
H	-1.647896000000	2.403566000000	9.690407000000
H	-1.968551000000	1.013415000000	8.641971000000
H	-0.328000000000	1.310778000000	9.244885000000

3b Ni(GaCp*)₃(PEt₃):

C	-2.664766000000	3.193906000000	-2.420832000000
C	-3.353665000000	2.540521000000	-3.502010000000
C	-2.669149000000	2.864041000000	-4.719138000000
C	-1.562433000000	3.704599000000	-4.392687000000
C	-1.555003000000	3.906226000000	-2.977924000000
Ga	-1.220801000000	1.531164000000	-3.298651000000
Ni	0.679531000000	0.447519000000	-3.864690000000
C	-4.619858000000	1.748460000000	-3.382735000000
C	-0.530456000000	4.705708000000	-2.235384000000
C	-3.062672000000	2.409003000000	-6.091177000000
C	-0.543702000000	4.262516000000	-5.335087000000
C	-3.102238000000	3.204124000000	-0.988083000000
Ga	2.180307000000	2.118587000000	-3.635258000000
C	3.677431000000	3.406664000000	-5.116279000000
C	4.320640000000	2.164825000000	-4.831275000000
C	4.557663000000	2.095093000000	-3.421894000000
C	4.052848000000	3.298275000000	-2.828751000000
C	3.501735000000	4.108107000000	-3.880373000000

C	4.688080000000	1.101600000000	-5.819050000000
C	2.962880000000	5.497372000000	-3.730641000000
C	5.217362000000	0.952049000000	-2.713093000000
C	4.152298000000	3.696898000000	-1.388004000000
C	3.302734000000	3.928281000000	-6.469456000000
P	0.580140000000	-0.292962000000	-5.861859000000
C	1.843817000000	-1.604734000000	-6.264281000000
C	-1.059685000000	-1.070101000000	-6.299491000000
C	0.826090000000	1.031096000000	-7.152173000000
C	-1.513559000000	-1.128315000000	-7.759901000000
H	-1.786964000000	-0.499588000000	-5.704568000000
H	-1.036914000000	-2.073985000000	-5.847274000000
H	4.054293000000	4.641597000000	-6.844804000000
H	2.338082000000	4.454421000000	-6.454899000000
H	3.228049000000	3.120776000000	-7.209457000000
H	6.300226000000	0.923425000000	-2.912309000000
H	4.799794000000	-0.015739000000	-3.029645000000
H	5.085541000000	1.023955000000	-1.626898000000
H	5.739460000000	1.186127000000	-6.138033000000
H	4.068657000000	1.157948000000	-6.724244000000
H	4.557967000000	0.098353000000	-5.389861000000
H	5.034223000000	4.332058000000	-1.206589000000
H	4.243791000000	2.821837000000	-0.731717000000
H	3.270598000000	4.264816000000	-1.059964000000
C	1.349872000000	0.672385000000	-8.543530000000
H	1.506186000000	1.744108000000	-6.667412000000
H	-0.140671000000	1.554200000000	-7.215172000000
H	3.753477000000	6.249604000000	-3.887105000000

H	2.548496000000	5.668298000000	-2.728463000000
H	2.167368000000	5.708443000000	-4.457960000000
C	1.605105000000	-2.582361000000	-7.417994000000
H	1.953474000000	-2.156822000000	-5.319999000000
H	2.791528000000	-1.061051000000	-6.395070000000
H	-3.826425000000	4.012809000000	-0.798331000000
H	-2.257441000000	3.356627000000	-0.303522000000
H	-3.588274000000	2.261359000000	-0.703334000000
H	-3.770977000000	3.107387000000	-6.565139000000
H	-3.547027000000	1.423294000000	-6.068609000000
H	-2.191524000000	2.329892000000	-6.755729000000
H	-5.508971000000	2.394794000000	-3.464579000000
H	-4.684525000000	1.229468000000	-2.416837000000
H	-4.698811000000	0.988151000000	-4.171660000000
H	-0.624657000000	5.357906000000	-5.417842000000
H	-0.651111000000	3.844859000000	-6.343663000000
H	0.478944000000	4.032728000000	-4.994133000000
H	-0.614071000000	5.781268000000	-2.456738000000
H	0.490994000000	4.396907000000	-2.511796000000
H	-0.628532000000	4.581990000000	-1.149611000000
H	-2.516463000000	-1.574256000000	-7.831510000000
H	-1.574619000000	-0.122748000000	-8.197048000000
H	-0.840085000000	-1.725783000000	-8.385322000000
H	2.430794000000	-3.306405000000	-7.480900000000
H	0.680798000000	-3.156394000000	-7.270105000000
H	1.534353000000	-2.076634000000	-8.387990000000
H	1.484534000000	1.582231000000	-9.146990000000
H	2.326912000000	0.173949000000	-8.484509000000

H	0.669126000000	0.009973000000	-9.090958000000
Ga	1.142812000000	-0.783440000000	-2.020739000000
C	-0.369914000000	-0.794701000000	-0.083089000000
H	-2.257984000000	-0.165408000000	0.751810000000
C	-1.823052000000	-0.469576000000	-0.212902000000
H	-2.399743000000	-1.325676000000	-0.584529000000
H	-1.983733000000	0.364349000000	-0.918168000000
C	0.237387000000	-2.079083000000	-0.231636000000
C	-0.471770000000	-3.376821000000	-0.473151000000
H	-0.755122000000	-3.863623000000	0.474050000000
H	0.159751000000	-4.085999000000	-1.025090000000
H	-1.391713000000	-3.234193000000	-1.055598000000
C	1.655130000000	-1.920614000000	-0.046489000000
C	2.666975000000	-3.025001000000	-0.001771000000
H	2.764988000000	-3.437136000000	1.015828000000
H	3.662510000000	-2.676331000000	-0.307759000000
H	2.390248000000	-3.857346000000	-0.662790000000
C	1.908848000000	-0.531044000000	0.221718000000
C	3.242308000000	0.069758000000	0.538913000000
H	3.442427000000	0.058608000000	1.622431000000
H	4.061027000000	-0.475271000000	0.050908000000
H	3.297719000000	1.116332000000	0.210417000000
C	0.659996000000	0.159067000000	0.186527000000
C	0.448521000000	1.633151000000	0.335375000000
H	0.064851000000	1.896169000000	1.334092000000
H	1.380582000000	2.191858000000	0.179585000000
H	-0.276906000000	2.001843000000	-0.405766000000

4b Ni(GaCp*)₄:

Ga	7.003808	10.582015	20.066590
C	8.444199	11.339933	21.891746
C	8.002036	12.425167	22.822763
H	8.859374	12.906544	23.317406
H	7.341388	12.039036	23.608231
H	7.452453	13.215129	22.283674
C	8.148839	9.943052	21.989786
C	7.458220	9.253021	23.126996
H	8.180382	8.920692	23.890228
H	6.736993	9.913984	23.625037
H	6.910116	8.362452	22.790795
C	8.755444	9.285640	20.852291
C	8.794618	7.805352	20.621666
H	9.641760	7.340420	21.151443
H	7.880030	7.312932	20.979169
H	8.904594	7.562911	19.556465
C	9.415474	10.289216	20.071035
C	10.150258	10.081147	18.783633
H	11.239585	10.170360	18.917495
H	9.950332	9.088334	18.361293
H	9.850507	10.827071	18.029931
C	9.214094	11.549534	20.709959
C	9.690822	12.877918	20.215874
H	9.899085	12.851364	19.137919
H	10.616581	13.192436	20.724924
H	8.935452	13.659090	20.381619
Ni	6.064722	12.097367	18.696974
Ga	5.164575	13.569713	20.139082

C	4.046393	14.285838	22.040889
C	3.390127	14.876104	20.895007
C	2.737066	13.823879	20.176921
C	2.990089	12.597081	20.862487
C	3.785734	12.877327	22.011670
Ga	7.519149	13.043119	17.264511
C	8.214618	14.202192	15.379177
C	8.811360	14.836467	16.533541
C	7.761768	15.466052	17.276114
C	6.530011	15.221047	16.596251
C	6.804835	14.453671	15.426542
Ga	4.531001	11.196233	17.318339
C	3.215442	9.481106	16.487764
C	3.874730	10.108477	15.363100
C	5.268447	9.796009	15.447660
C	5.474332	8.993075	16.608307
C	4.214955	8.789990	17.247782
C	10.280191	14.914206	16.820359
C	8.964376	13.528976	14.269837
C	5.771474	13.984792	14.450508
C	5.171894	15.655410	17.047226
C	7.898206	16.209361	18.567733
C	1.735735	9.453081	16.724168
C	3.186953	10.836682	14.248174
C	6.356039	10.251177	14.525662
C	6.799837	8.488011	17.081811
C	4.002659	8.023676	18.516055
C	3.313280	16.343178	20.598942

C	4.746240	15.042219	23.128958
C	4.272070	11.849972	22.985763
C	2.536274	11.237512	20.435556
C	1.967091	13.951721	18.900328
H	10.747330	15.760303	16.290938
H	10.806600	14.003846	16.502302
H	10.477676	15.051031	17.891495
H	9.287276	14.256258	13.507414
H	8.348756	12.774745	13.762353
H	9.867482	13.023360	14.637428
H	6.197902	13.293327	13.713750
H	5.328876	14.827004	13.896654
H	4.946134	13.461861	14.960122
H	4.849410	16.577743	16.537080
H	5.155620	15.851820	18.127641
H	4.418285	14.880809	16.846974
H	8.893322	16.072795	19.009329
H	7.158412	15.859556	19.306845
H	7.740566	17.290666	18.433344
H	2.829625	10.137432	13.474947
H	3.858094	11.552803	13.756637
H	2.312557	11.397467	14.605490
H	1.258179	8.625089	16.175642
H	1.252376	10.382036	16.392261
H	1.496630	9.318857	17.787446
H	7.104790	7.577702	16.540120
H	6.774281	8.242079	18.151984
H	7.587423	9.241581	16.939835

H	3.018445	8.233185	18.953577
H	4.761375	8.286577	19.270579
H	4.067032	6.936807	18.351379
H	5.973266	10.927902	13.752363
H	6.834075	9.400985	14.015695
H	7.148040	10.787082	15.075429
H	4.036164	15.378222	23.901884
H	5.505864	14.426694	23.628477
H	5.251040	15.937748	22.742133
H	2.487509	16.820297	21.151075
H	4.236864	16.865923	20.883141
H	3.143246	16.532843	19.531089
H	1.625058	10.925261	20.971394
H	2.312488	11.212136	19.360368
H	3.311030	10.480947	20.623394
H	2.093274	14.944099	18.449620
H	2.303345	13.207720	18.158864
H	0.889087	13.792942	19.057552
H	4.981396	12.279552	23.703360
H	3.440722	11.415326	23.561904
H	4.780159	11.018299	22.471325

5 Ni(PEt₃)₄:

Ni	-0.091096000000	0.022551000000	-0.150607000000
P	0.500405000000	0.794405000000	1.841995000000
P	-2.288480000000	0.332762000000	-0.255976000000
P	0.707868000000	1.027013000000	-1.964213000000

P	0.670736000000	-2.076049000000	-0.001672000000
C	2.439620000000	1.749671000000	-2.007178000000
H	2.487968000000	2.448833000000	-2.858562000000
H	2.550603000000	2.350292000000	-1.093232000000
C	0.716760000000	0.182364000000	-3.651795000000
H	-0.276319000000	0.393411000000	-4.073197000000
H	1.438547000000	0.721831000000	-4.286320000000
C	-0.134289000000	2.551513000000	-2.671604000000
H	0.341761000000	2.747669000000	-3.646389000000
H	-1.170640000000	2.257957000000	-2.889644000000
C	-0.099977000000	3.810143000000	-1.815782000000
H	-0.645595000000	4.632889000000	-2.300304000000
H	-0.557173000000	3.636395000000	-0.837114000000
H	0.929493000000	4.153620000000	-1.646304000000
C	3.569913000000	0.730001000000	-2.113163000000
H	4.552108000000	1.220991000000	-2.060613000000
H	3.523530000000	-0.006023000000	-1.303585000000
H	3.525809000000	0.181735000000	-3.064001000000
C	0.964250000000	-1.317720000000	-3.694526000000
H	0.290174000000	-1.831412000000	-2.998489000000
H	0.784927000000	-1.720510000000	-4.702011000000
H	1.991965000000	-1.577940000000	-3.413041000000
C	0.843245000000	-2.967115000000	1.657043000000
H	1.628987000000	-3.725204000000	1.510128000000
H	1.242465000000	-2.244118000000	2.381738000000
C	2.438345000000	-2.429365000000	-0.549873000000
H	2.551586000000	-1.954604000000	-1.531548000000
H	2.508173000000	-3.517555000000	-0.711584000000

C	-0.032289000000	-3.538618000000	-0.961651000000
H	0.478175000000	-3.542318000000	-1.934441000000
H	0.302005000000	-4.451314000000	-0.442316000000
C	-0.391290000000	-3.656697000000	2.233395000000
H	-0.138570000000	-4.170528000000	3.172149000000
H	-4.117086000000	-2.052263000000	0.827604000000
H	-0.794659000000	-4.410789000000	1.544912000000
C	3.561690000000	-1.983529000000	0.379910000000
H	3.521430000000	-2.499582000000	1.348325000000
H	4.542324000000	-2.202673000000	-0.066639000000
H	3.521687000000	-0.908227000000	0.574843000000
C	-1.538724000000	-3.547051000000	-1.174693000000
H	-1.866789000000	-4.480725000000	-1.654628000000
H	-2.090764000000	-3.438200000000	-0.232566000000
H	-1.831002000000	-2.714718000000	-1.823253000000
C	-0.424563000000	-0.105632000000	3.205022000000
H	-1.399807000000	0.400267000000	3.251517000000
H	-0.634630000000	-1.108844000000	2.823113000000
C	0.157973000000	2.513405000000	2.500243000000
H	0.431709000000	2.537541000000	3.566791000000
H	-0.934817000000	2.611495000000	2.459891000000
C	2.257287000000	0.598463000000	2.453849000000
H	2.460977000000	-0.481598000000	2.455417000000
H	2.315708000000	0.933055000000	3.499948000000
C	0.185005000000	-0.187898000000	4.604854000000
H	1.106817000000	-0.784429000000	4.611712000000
H	0.427820000000	0.803041000000	5.013241000000
H	-0.518823000000	-0.664697000000	5.302599000000

C	0.823303000000	3.669573000000	1.751739000000
H	0.271671000000	4.609925000000	1.893077000000
H	1.848980000000	3.839675000000	2.100365000000
H	0.870528000000	3.467725000000	0.674439000000
C	3.306471000000	1.320257000000	1.609188000000
H	4.322282000000	0.990679000000	1.869729000000
H	3.148459000000	1.125645000000	0.542058000000
H	3.265642000000	2.406158000000	1.750736000000
C	-2.974659000000	2.048815000000	-0.594514000000
H	-2.520489000000	2.409207000000	-1.524825000000
H	-4.051319000000	1.925262000000	-0.794809000000
C	-2.771918000000	3.077666000000	0.512771000000
H	-3.271665000000	2.777770000000	1.443940000000
H	-1.708534000000	3.214190000000	0.734011000000
H	-3.178766000000	4.055822000000	0.219411000000
C	-3.337451000000	-0.536644000000	-1.540135000000
H	-3.386629000000	-1.593170000000	-1.251335000000
H	-4.362995000000	-0.139201000000	-1.466946000000
C	-2.806028000000	-0.411225000000	-2.963614000000
H	-1.782333000000	-0.801319000000	-3.023789000000
H	-3.428413000000	-0.970362000000	-3.676746000000
H	-2.780351000000	0.635640000000	-3.297251000000
C	-3.402253000000	-0.025110000000	1.206230000000
H	-2.995352000000	0.538194000000	2.056400000000
H	-4.398596000000	0.396499000000	0.993579000000
C	-3.509964000000	-1.504578000000	1.560212000000
H	-1.199652000000	-2.952145000000	2.458282000000
H	-2.515731000000	-1.966541000000	1.571554000000

H -3.966701000000 -1.653781000000 2.548522000000

EDA-NOCV Energies for $[\text{Ni}(\text{ECp}^*)_n(\text{PET}_3)_{4-n}]$

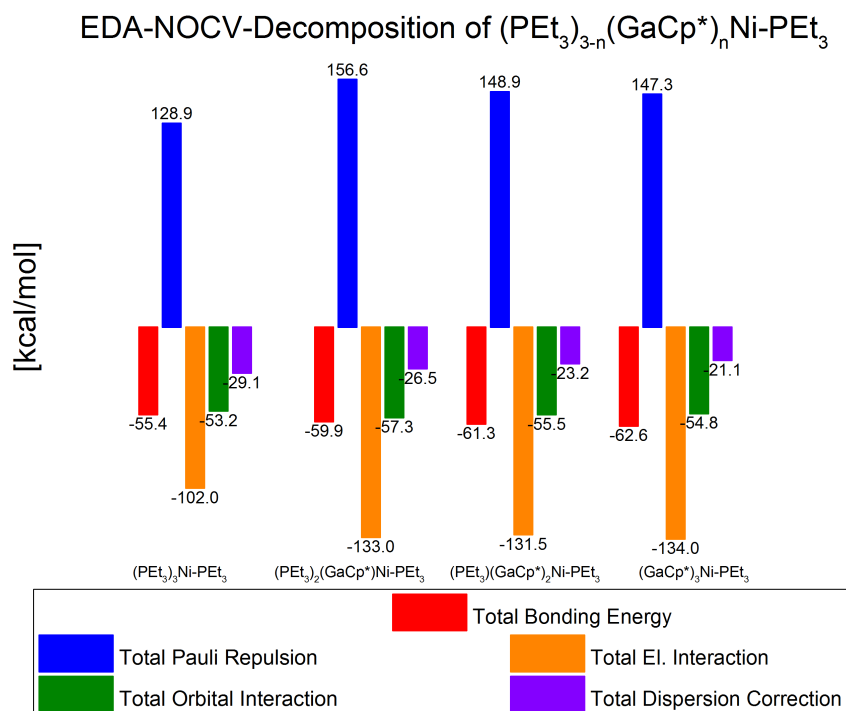


Figure S34: EDA-NOCV Decomposition investigating the Ni-PET₃ bonding in heteroleptic NiGaP complexes.

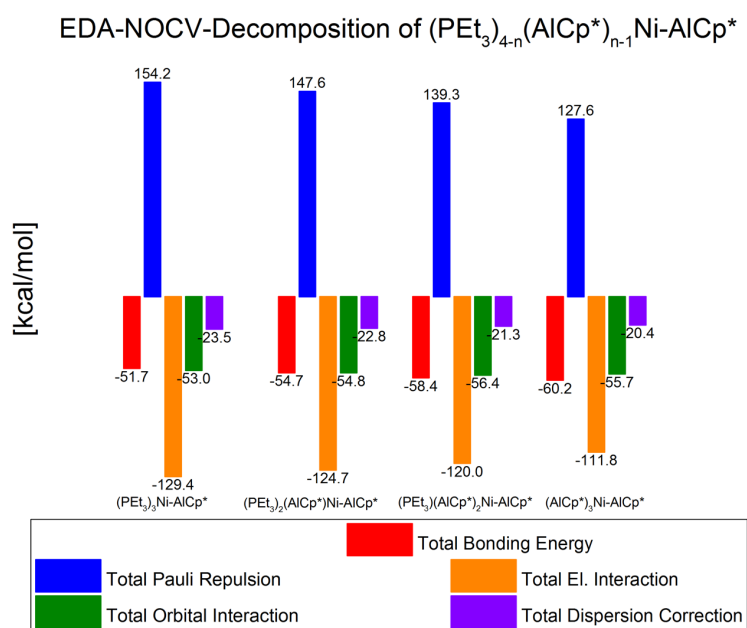


Figure S35: EDA-NOCV Decomposition investigating the Ni-AlCp* bonding in heteroleptic NiAlP complexes.

EDA-NOCV-Decomposition of $(\text{PEt}_3)_{3/4-n}(\text{GaCp}^*)_{n-1}\text{Ni-GaCp}^*$

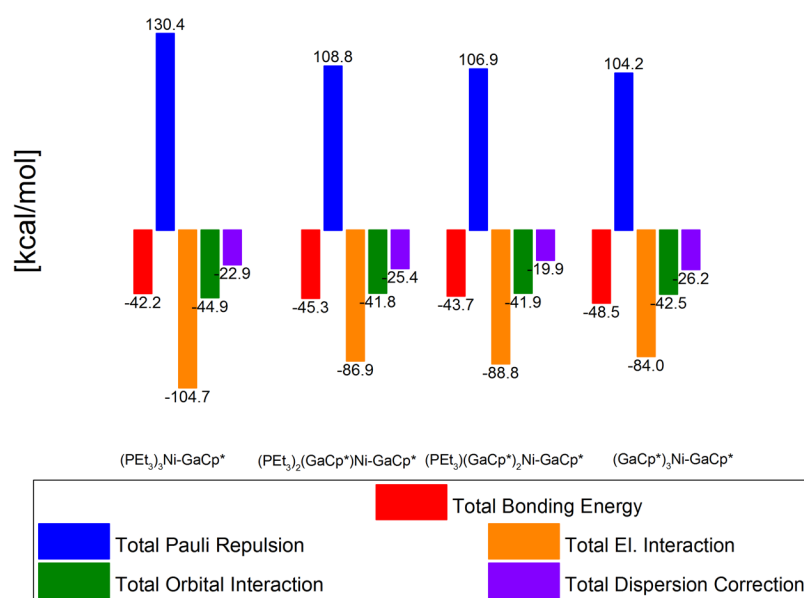
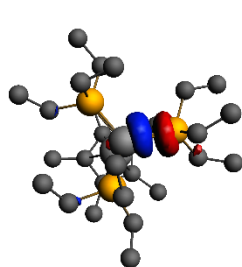


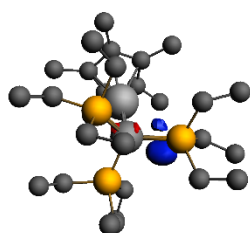
Figure S36: EDA-NOCV Decomposition investigating the Ni-GaCp* bonding in heteroleptic NiGaP complexes.

EDA-NOCV derived Deformation Densities:

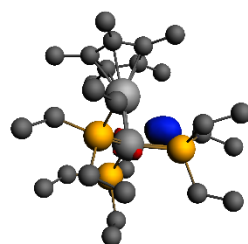
1a:



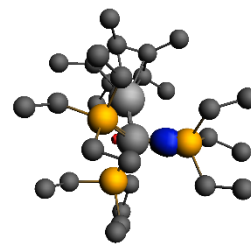
$\nu = -0.4943$, $\Delta E_{\text{orb}} = -$
22.53 kcal/mol



$\nu = -0.3451$, $\Delta E_{\text{orb}} = -$
11.61 kcal/mol

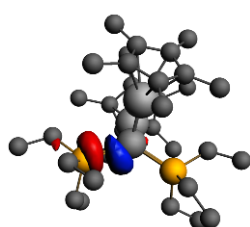


$\nu = -0.3376$, $\Delta E_{\text{orb}} = -$
11.59 kcal/mol

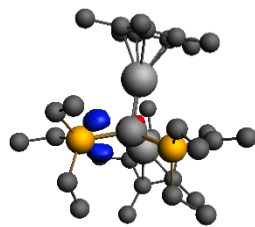


$\nu = -0.1827$, $\Delta E_{\text{orb}} = -$
6.43 kcal/mol

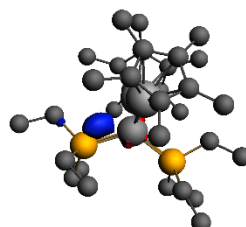
2a:



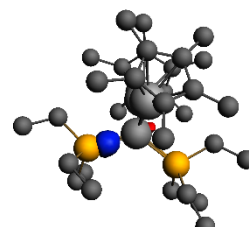
$\nu = -0.4997$, $\Delta E_{\text{orb}} = -$
23.39 kcal/mol



$\nu = -0.3688$, $\Delta E_{\text{orb}} = -$
12.78 kcal/mol

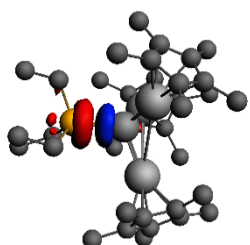


$\nu = -0.3457$, $\Delta E_{\text{orb}} = -$
11.66 kcal/mol

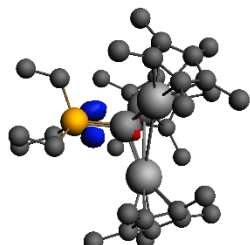


$\nu = -0.1718$, $\Delta E_{\text{orb}} = -$
6.03 kcal/mol

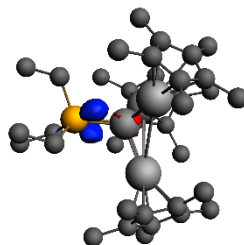
3a:



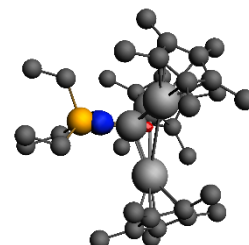
$\nu = -0.5376$, $\Delta E_{\text{orb}} = -$
25.43 kcal/mol



$\nu = -0.3436$, $\Delta E_{\text{orb}} = -$
11.22 kcal/mol

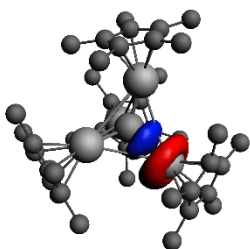


$\nu = -0.3430$, $\Delta E_{\text{orb}} = -$
11.20 kcal/mol

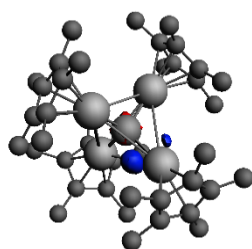


$\nu = -0.1582$, $\Delta E_{\text{orb}} = -$
5.36 kcal/mol

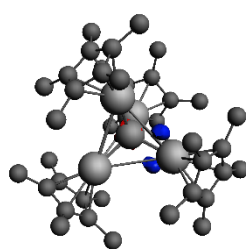
4a:



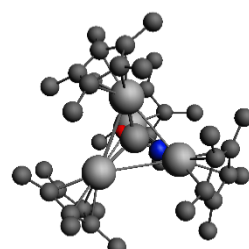
$\nu = -0.6149$, $\Delta E_{\text{orb}} = -$
28.24 kcal/mol



$\nu = -0.3451$, $\Delta E_{\text{orb}} = -$
9.37 kcal/mol

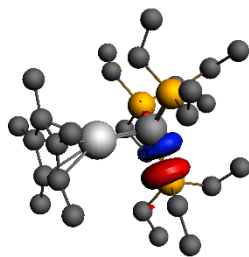


$\nu = -0.3374$, $\Delta E_{\text{orb}} = -$
9.06 kcal/mol

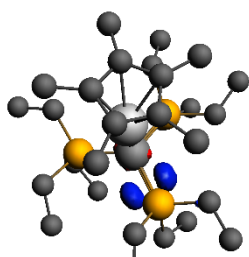


$\nu = -0.1752$, $\Delta E_{\text{orb}} = -$
4.75 kcal/mol

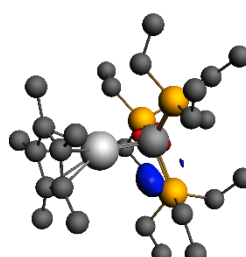
1b:



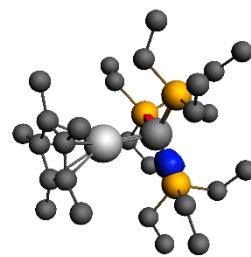
$\nu = -0.4775$, $\Delta E_{\text{orb}} = -$
21.73 kcal/mol



$\nu = -0.3441$, $\Delta E_{\text{orb}} = -$
11.90 kcal/mol

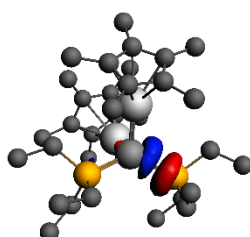


$\nu = -0.3383$, $\Delta E_{\text{orb}} = -$
11.31 kcal/mol

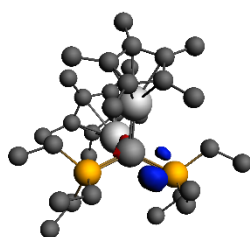


$\nu = -0.1833$, $\Delta E_{\text{orb}} = -$
6.62 kcal/mol

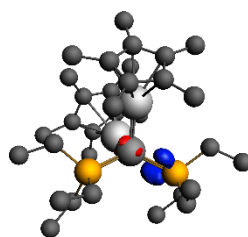
2b:



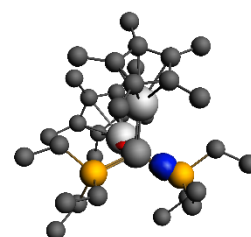
$\nu = -0.4801$, $\Delta E_{\text{orb}} = -$
21.74 kcal/mol



$\nu = -0.3517$, $\Delta E_{\text{orb}} = -$
11.84 kcal/mol

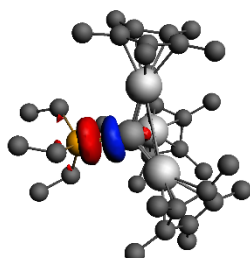


$\nu = -0.3284$, $\Delta E_{\text{orb}} = -$
10.62 kcal/mol

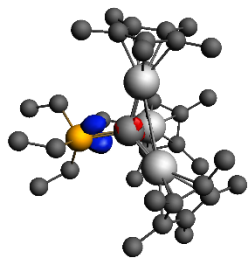


$\nu = -0.1870$, $\Delta E_{\text{orb}} = -$
6.88 kcal/mol

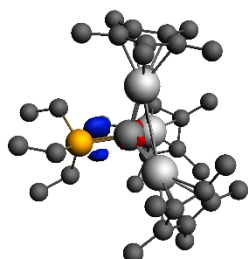
3b:



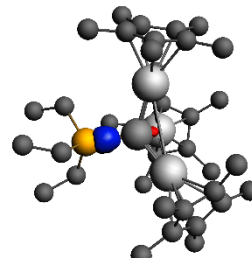
$\nu = -0.5331$, $\Delta E_{\text{orb}} = -$
24.66 kcal/mol



$\nu = -0.3517$, $\Delta E_{\text{orb}} = -$
10.44 kcal/mol

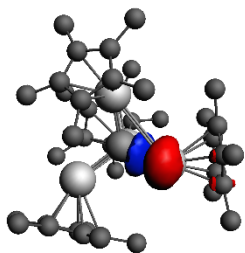


$\nu = -0.3284$, $\Delta E_{\text{orb}} = -$
10.40 kcal/mol

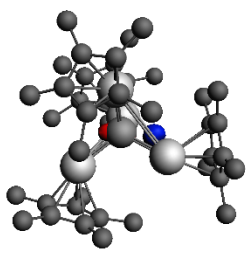


$\nu = -0.1870$, $\Delta E_{\text{orb}} = -$
6.31 kcal/mol

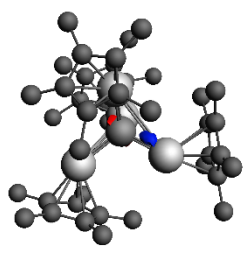
4b:



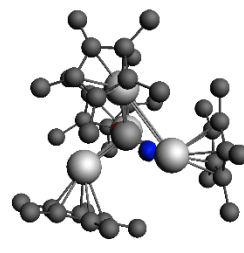
$\nu = -0.4656$, $\Delta E_{\text{orb}} = -$
18.05 kcal/mol



$\nu = -0.3204$, $\Delta E_{\text{orb}} = -$
8.2144 kcal/mol



$\nu = -0.2917$, $\Delta E_{\text{orb}} = -$
6.78 kcal/mol



$\nu = -0.1826$, $\Delta E_{\text{orb}} = -$
4.57 kcal/mol

5:

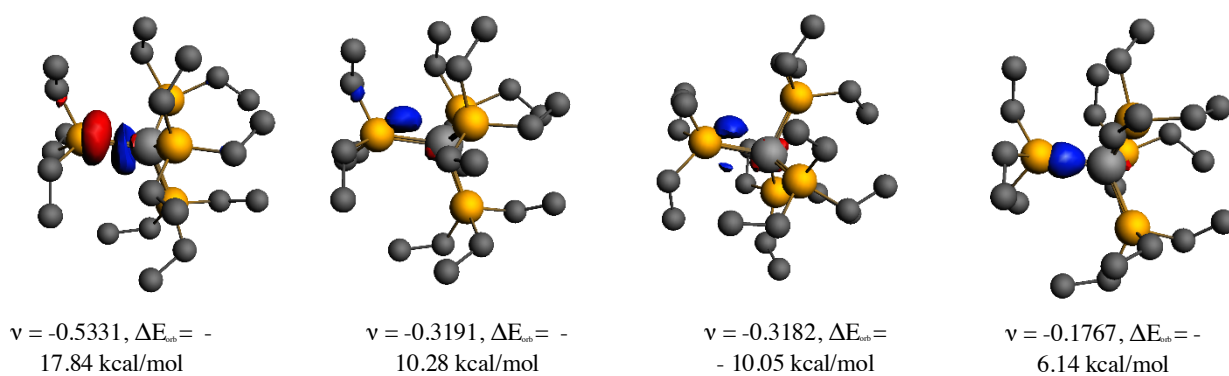


Figure S37: Deformation Densities found for $[\text{Ni}(\text{ECp}^*)_n(\text{PEt}_3)_{4-n}]$. From left to right: σ -type interaction, π -type interaction, π -type interaction, σ_{back} -type interaction. Charge flow from red to blue regions.