Electronic Supplementary Information

From zinco(II) arsaketenes to silylene-stabilised zinco arsinidene complexes

1. Experimental Section

Materials and methods: All manipulations were carried out using standard Schlenk and glovebox techniques under a dry atmosphere of nitrogen. The compounds $LZnCl_2Li(OEt_2)_2$ (**1**),[1] $NaAsCO(dioxane)_{2,3}$,[2] [C(Me)N(*i*Pr)]$_2$C: (NHC),[3] [C(H)N(*t*Bu)]$_2$Si: (*t*BuNHSi),[4] and [C(H)N(2,6-*i*Pr$_2$-C_6H_3)]$_2$Si: (DippNHSi)[5] were prepared according with the literature procedures. Ambient temperature is referred to an interval between 20 °C and 30 °C. Toluene, hexane, tetrahydrofuran, diethyl ether, THF-d_8 and C_6D_6 were dried with the sodium-benzophenone mixture and stored under molecular sieves prior use. ^{1}H-, ^{13}C{^{1}H}-, ^{29}Si{^{1}H}- and 2D- NMR spectra were recorded with Bruker spectrometers AV200, AV400 and AV500. The spectra were referenced to $SiMe_4$ using the residual solvent signals as internal standards, or externally to $SiMe_4$ in the case of the ^{29}Si{^{1}H}-NMR. Abbreviations: s = singlet; d = doublet; t = triplet; sept = septet; m = multiplet. IR spectra were measured from powder samples inside a nitrogen filled glovebox using a Thermofisher Nicolet iS5 IR Spectrometer (ATR-Diamond). Melting points were determined in sealed glass capillaries under nitrogen. Elemental analyses were performed by the analytical laboratory service in the Institute of Chemistry, Technical University of Berlin, Germany.

1.1. Synthesis and selected spectroscopic data of the compounds reported

1.1.1. Synthesis of LZnCl(NHC) (3)

Compound **1** (1.68 g, 2.4 mmol), NHC (0.45 g, 2.5 mmol) and a magnetic stir bar were mixed in a 100 mL Schlenk flask in the glovebox. To this mixture, toluene at -78°C (50 mL) was added. The resulting suspension was stirred and warmed up to ambient temperature in an 18 h period. The mixture was cannula filtered and the solvent was removed under vacuum. The residual white solid was washed with Et_2O (1 x 4 mL), hexane (1 x 4 mL) and dried under vacuum. Yield: 1.00 g (60 %), m.p. 252 °C. Single crystals suitable for X-ray diffraction analysis were obtained from a saturated solution of **3** in toluene at ambient temperature after 18 hours. Elemental analysis calcd (%) for $C_{40}H_{61}N_4ClZn$: C 68.75, H 8.80, N 8.02; found: C 69.37, H 9.20, N 8.28. ^{1}H NMR (THF-d_8, 500 MHz, 298 K): δ (ppm) = 0.63 (d, $^3J_{HH}$ = 6.7 Hz, 6H, L-*i*Pr-C*H*$_3$), 1.98 (d, $^3J_{HH}$ = 6.8 Hz, 6H, L-*i*Pr-C*H*$_3$), 1.11 (d, $^3J_{HH}$ = 6.8 Hz, 6H, L-*i*Pr-C*H*$_3$), 1.17 (d, $^3J_{HH}$ = 7.0 Hz, 6H, NHC-*i*Pr-C*H*$_3$), 1.33 (d, $^3J_{HH}$ = 6.7 Hz, 6H, L-*i*Pr-C*H*$_3$), 1.60 (d, $^3J_{HH}$ = 6.8 Hz, 6H, NHC-*i*Pr-C*H*$_3$), 1.67 (s, 6H, L-NC*Me*), 2.20 (s, 3H, NHC-NC*Me*), 2.34 (s, 3H, NHC-NC*Me*), 3.00 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, L-*i*Pr-C*H*), 3.57 (sept, $^3J_{HH}$ = 6.7 Hz, 2H, L-*i*Pr-C*H*), 4.85 (s, 1H, L-NCC*H*CN), 5.28 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, NHC-*i*Pr-C*H*), 6.12 (sept, $^3J_{HH}$ = 7.0 Hz, 1H, NHC-*i*Pr-C*H*), 6.92-7.10 (m, 6 H, *m* and *p* Ar*H*). ^{13}C{^{1}H}-NMR (THF-d_8, 125 MHz, 298 K): δ (ppm) = 10.54 and 10.61 (NHC-C*Me*), 22.19 and 23.17 (NHC-*i*Pr-*C*H$_3$), 24.55 (L-NC*Me*), 24.76, 25.10, 25,20 and 25.51 (L-*i*Pr-*C*H$_3$) 27.72 and 29.01 (L-*i*Pr-*C*H), 51.90 and 54.32 (NHC-*i*Pr-*C*H), 94.12 (L-NC*C*HCN), 123.48, 124.48 and 125.22 (L *m* and *p* -Ar*C*), 126.89 and

127.89 (L *o*-Ar*C*), 142.71 and 144.54 (NHC -N*C*Me), 146.34 (L *i*-Ar*C*), 167.58 (L-NCC*H*CN), 176.78 (NHC-N*C*:N).

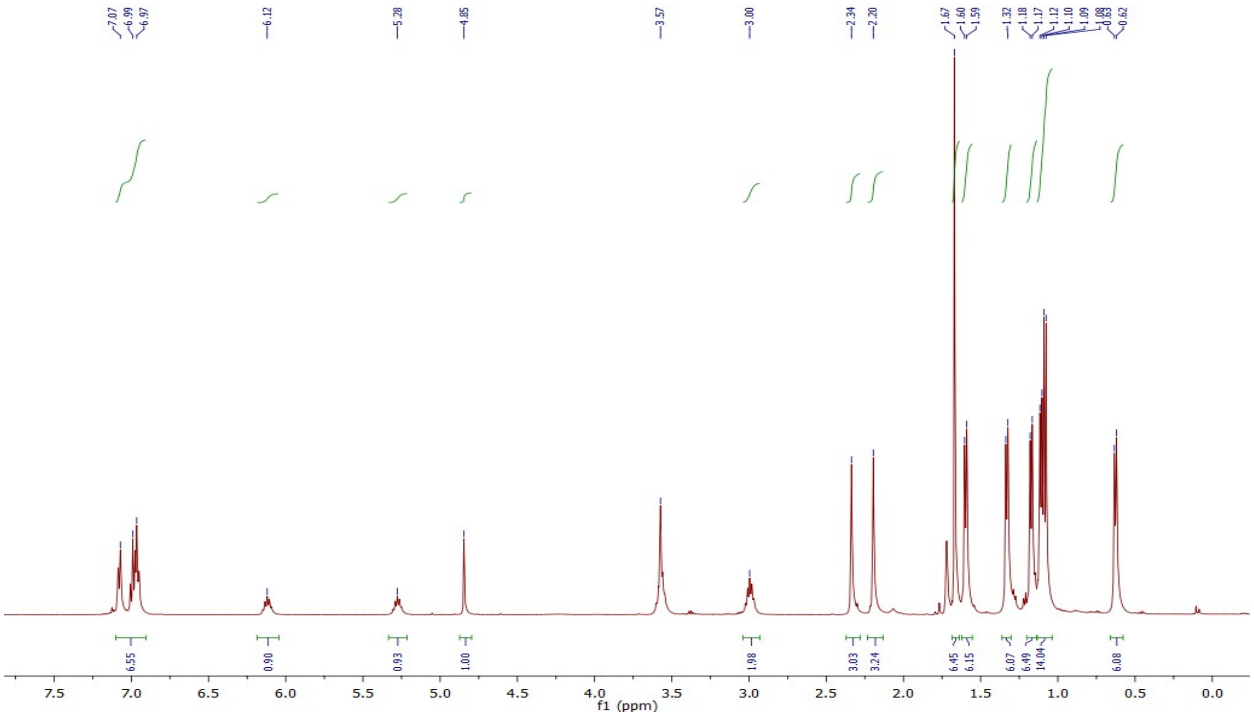

Figure S1. ^{1}H-NMR spectrum of **3** in THF-d_8 at 298 K.

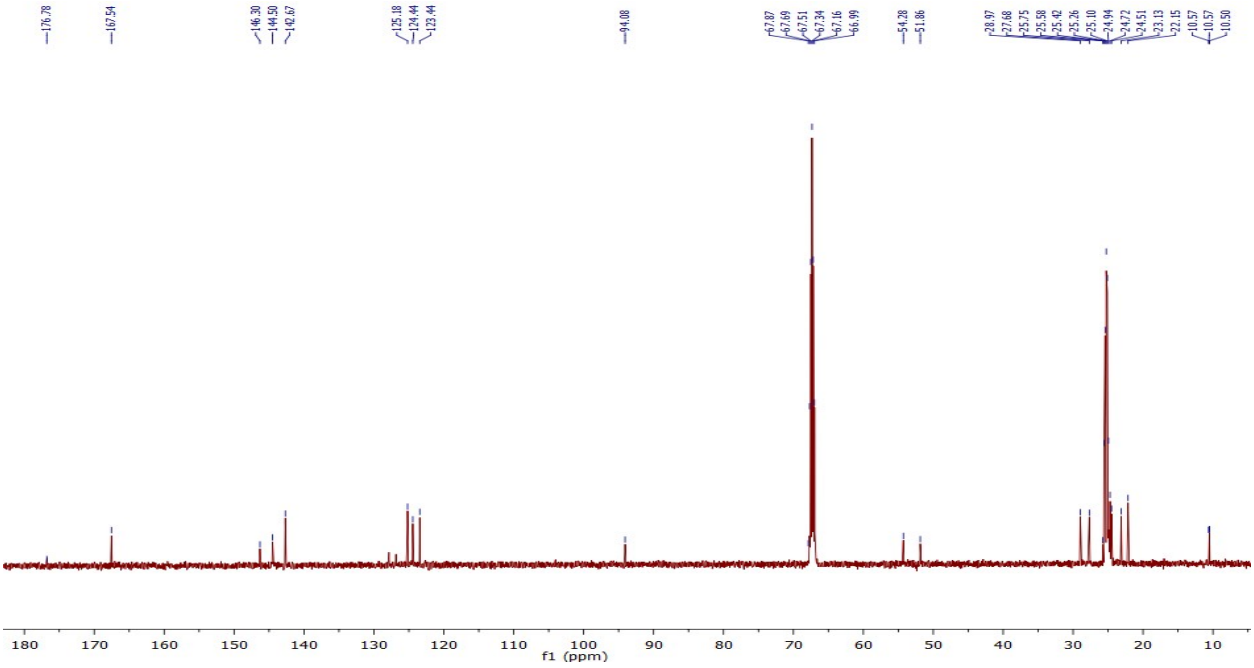

Figure S2. ^{13}C{^{1}H}-NMR spectrum of **3** in THF-d_8 at 298 K.

1.1.2. Synthesis of LZn(AsCO)(*i*PrNHC) (4)

A THF (30 mL) solution of **3** (1.80 g, 2.6 mmol) at ambient temperature was added dropwise over a THF (30 mL) solution of $NaAsCO(dioxane)_{2,3}$ (0.93 g, 2.8 mmol, 1.1 eq.) precooled at -78 °C. The mixture was stirred and warm up to ambient temperature in two hours. After this, the mixture was a yellow solution mixed with a white solid. The volatiles were removed under vacuum. The remained yellow residue was extracted with Et_2O (150 mL). This mixture was filtered over celite and the yellow solution was concentrated until incipient crystal formation; at this point, the mixture was kept at -28 °C for 40 hours. The crystalline solid was separated via Teflon-cannula filtration, washed with hexane (1 x 7 mL) and dried under vacuum. Yield: 0.60 g (30 %), m.p. 136 °C (d.). Elemental analysis calcd (%) for $C_{41}H_{61}N_4AsOZn$: C 64.27, H 8.02, N 7.31; found: C 64.87, H 8.09, N 7.38. ^{1}H NMR (C_6D_6, 200 MHz, 298 K): δ (ppm) = 0.77 (d, $^3J_{HH}$ = 6.8 Hz, 6H, NHC-*i*Pr-C*H*$_3$), 1.09 (d, $^3J_{HH}$ = 6.7 Hz, 6H, L-*i*Pr-C*H*$_3$), 1.13 (d, $^3J_{HH}$ = 6.9 Hz, 6H, L-*i*Pr-C*H*$_3$), 1.32 (d, $^3J_{HH}$ = 6.9 Hz, 12H, L-*i*Pr-C*H*$_3$), 1.56 (s, 3H, NHC-NC*Me*), 1.69 (s, 6H, L-NC*Me*), 1.71 (s, 3H, NHC-NC*Me*), 1.76 (d, $^3J_{HH}$ = 6.8 Hz, 6H, NHC-*i*Pr-C*H*$_3$), 3.02 (sept, $^3J_{HH}$ = 6.9 Hz, 2H, L-*i*Pr-C*H*), 3.87 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, L-*i*Pr-C*H*), 4.80 (s, 1H, L-NCC*H*CN), 5.35 (sept, $^3J_{HH}$ = 6.9 Hz, 1H, NHC-*i*Pr-C*H*), 6.85 (sept, $^3J_{HH}$ = 6.9 Hz, 1H, NHC-*i*Pr-C*H*), 7.04-7.34 (m, 6 H; *m* and *p* Ar*H*). ^{13}C{^{1}H}-NMR (C_6D_6, 50 MHz, 298 K): δ (ppm) = 177.29 (As*C*O), 185.01 (free *C*O). IR(cm^{-1}): 1862 (AsCO).

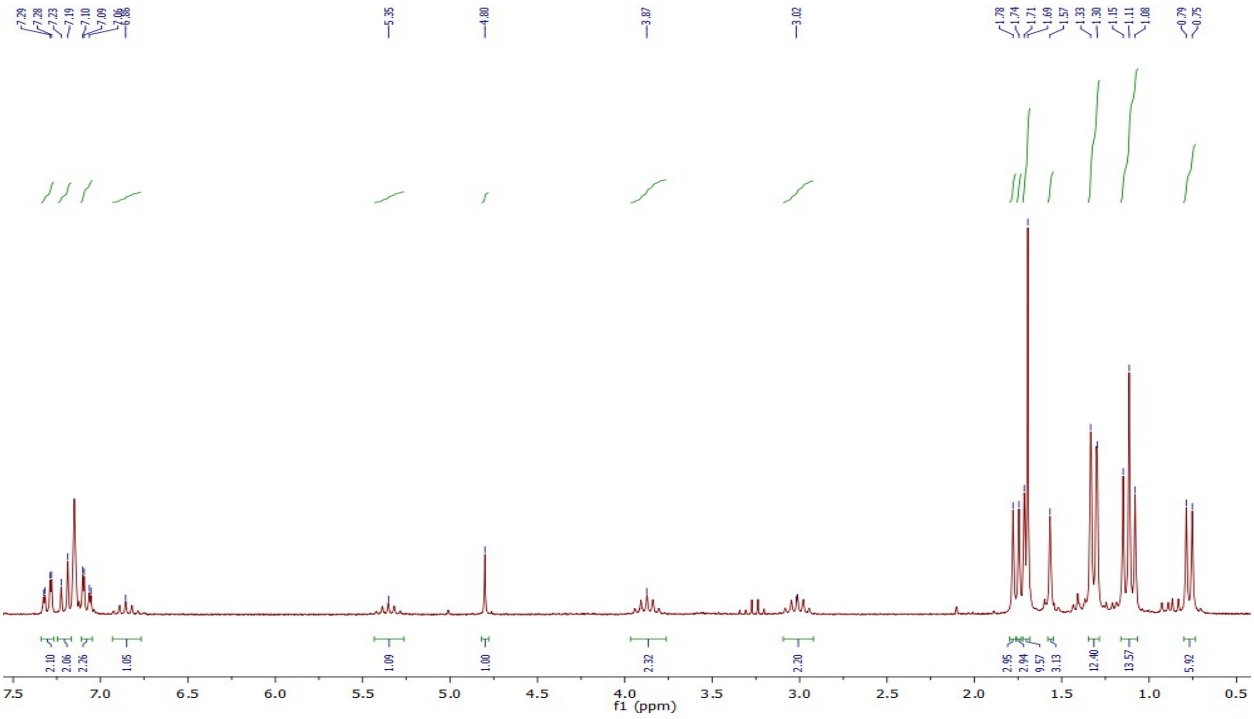

Figure S3. ^{1}H-NMR spectrum of **4** in C_6D_6 at 298 K.

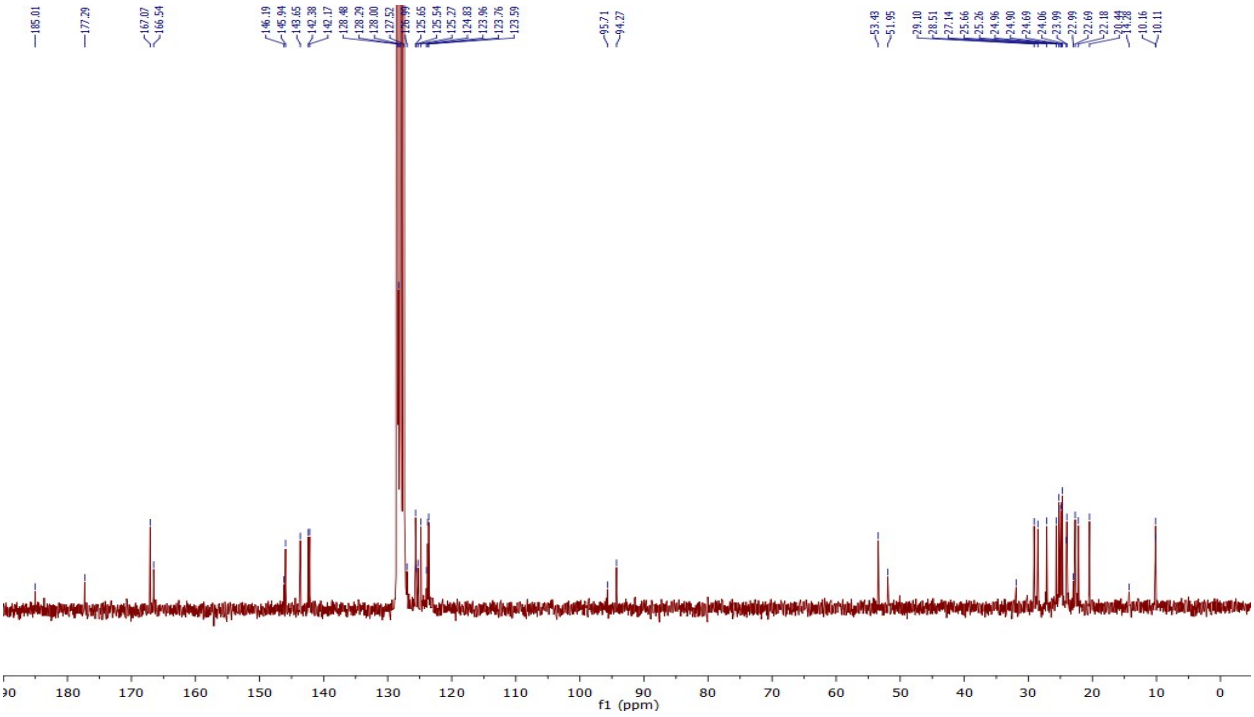

Figure S4. $^{13}C\{^{1}H\}$-NMR spectrum of **4** in C_6D_6 at 298 K.

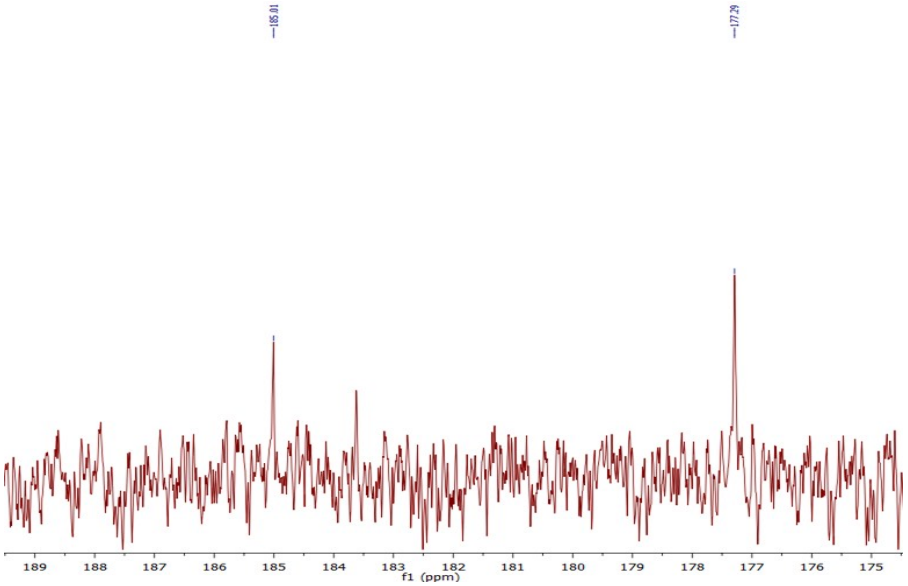

Figure S5. Amplified $^{13}C\{^{1}H\}$-NMR spectrum of **4** in C_6D_6 at 298 K. There is CO in solution.

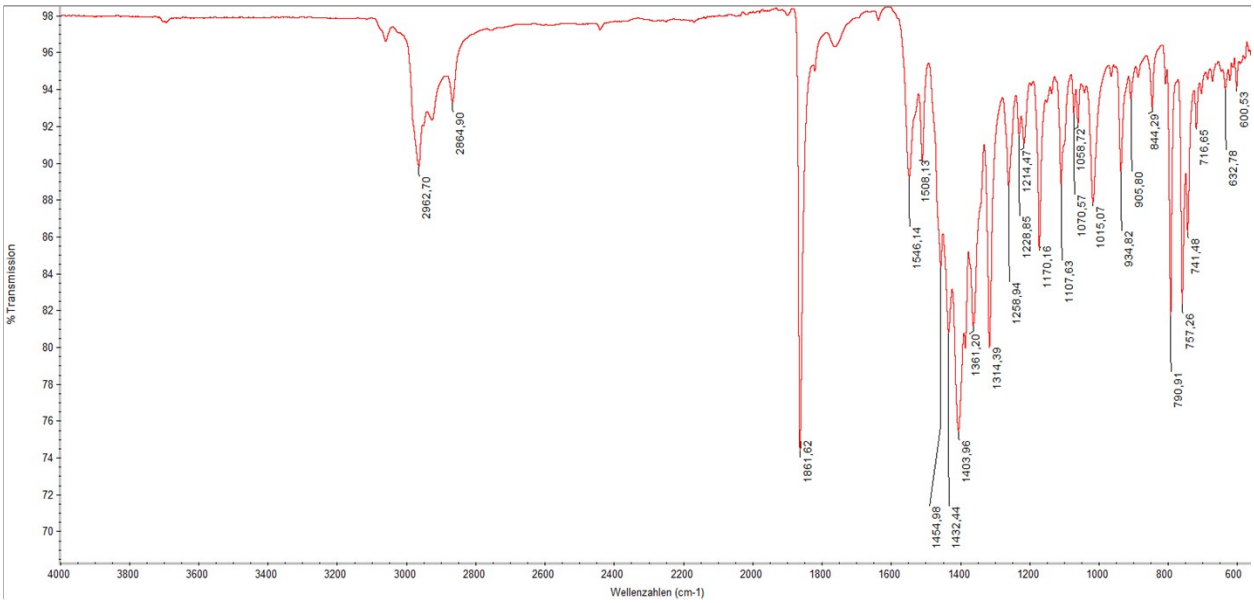

Figure S6. IR (ATR) spectrum of **4**.

1.1.3. Synthesis of [NHC→^{t}BuNHSi→AsZnL] (5)

Compound **4** (0.19 g, 0.25 mmol), ^{t}BuNHSi (0.050 g, 0.25 mmol) and a magnetic stir bar were mixed in a 25 mL Schlenk flask in the glovebox. To this mixture, toluene at ambient temperature (10 mL) was added. The resulting yellow-orange solution was stirred at ambient temperature for two days. After this time, the mixture was a dark solution containing a small amount of black powder. The mixture was filtered and the solution was concentrated until the incipient formation of orange crystals. The mixture was layered with hexane (8 mL) and kept at ambient temperature for one week. **5** was isolated after filtration, washing with hexane (2 mL) and drying under vacuum. Yield: 0.050 g (21 %), m.p. 170 °C. Elemental analysis calcd (%) for $C_{50}H_{81}N_6AsSiZn$: C 64.26, H 8.74, N 8.99; found: C 63.46, H 8.87, N 9.07. ^{1}H NMR (C_6D_6, 200 MHz, 298 K): δ (ppm) = 1.15 (d, $^{3}J_{HH}$ = 6.9 Hz, 12H, NHC-^{i}Pr-CH_3), 1.30 (d, $^{3}J_{HH}$ = 6.9 Hz, 6H, L-^{i}Pr-CH_3), 1.33 (s, 18H, NHSi-^{t}Bu-CH_3), 1.50 (s, 6H, NHC-^{i}Pr-C*Me*), 1.69 (d, $^{3}J_{HH}$ = 6.8 Hz, 12H, L-^{i}Pr-CH_3), 1.75 (s, 6H, L-NC*Me*), 3.57 (sept, $^{3}J_{HH}$ = 6.9 Hz, 4H, L-^{i}Pr-C*H*), 5.05 (s, 1H, L -NCC*H*CN), 5.69 (s, 2H, NHSi-NC*H*), 7.03 (sept, $^{3}J_{HH}$ = 6.9 Hz, 2H, NHC-^{i}Pr-C*H*), 7.26 (s, 6 H; *m* and *p* Ar*H*). ^{13}C{^{1}H}-NMR (C_6D_6, 50 MHz, 298 K): δ (ppm) = 10.45 (NHC-C*Me*), 21.81 (NHC-^{i}Pr-*C*H_3), 24.31 (L-NC*Me*), 24.59 and 25.95 (L-^{i}Pr- *C*H_3), 28.74 (L-^{i}Pr-*C*H), 31.24 (NHSi-^{t}Bu-*C*H_3), 48.77 (NHC-^{i}Pr-*C*H), 52.88 (NHSi-^{t}Bu-*C*Me_3), 95.61 (L-NC*C*HCN), 111.90 (NHSi-NCH), 123.56, 125.13 and 126.60 (L *m* and *p* -Ar*C*), 128.28 (L *o*-Ar*C*), 142.75 (NHC-*C*Me), 147.02 (L *i*-Ar*C*), 156.64 (NHC-NC:N), 166.55 (L-NCCHCN). ^{29}Si{^{1}H}-NMR (C_6D_6, 79 MHz, 298 K) δ (ppm) = -6.31.

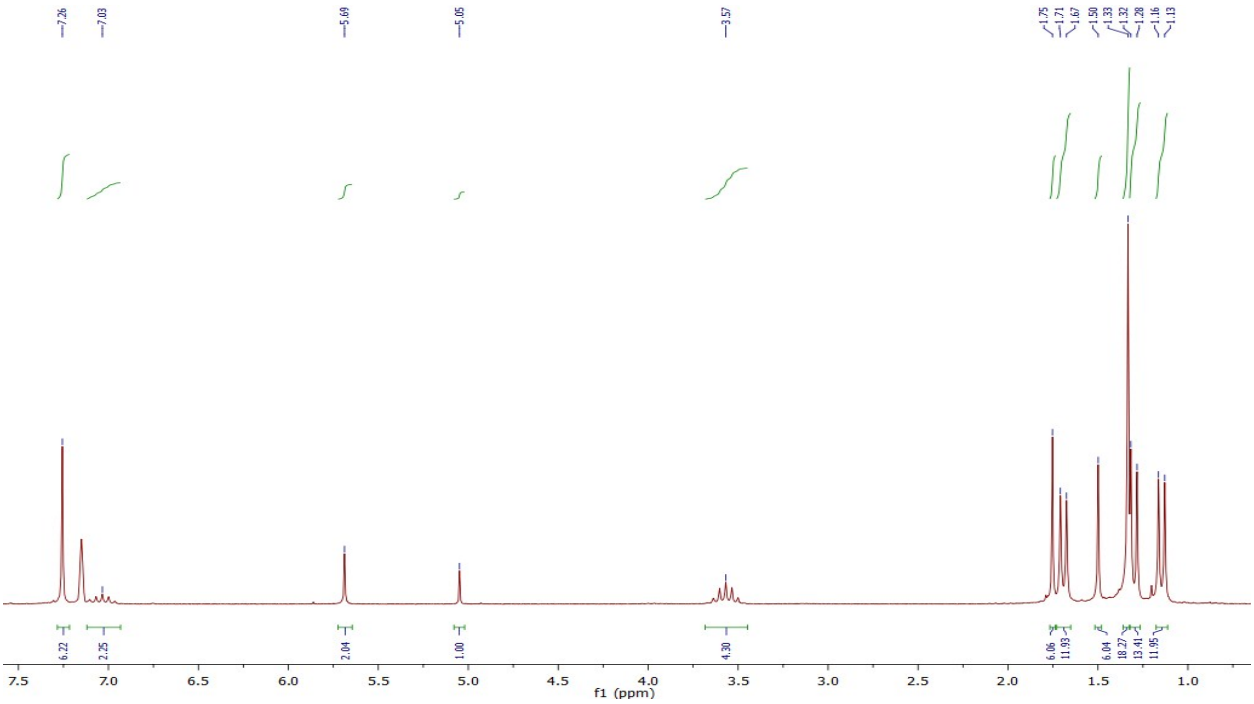

Figure S7. ^{1}H-NMR spectrum of **5** in C_6D_6 at 298 K.

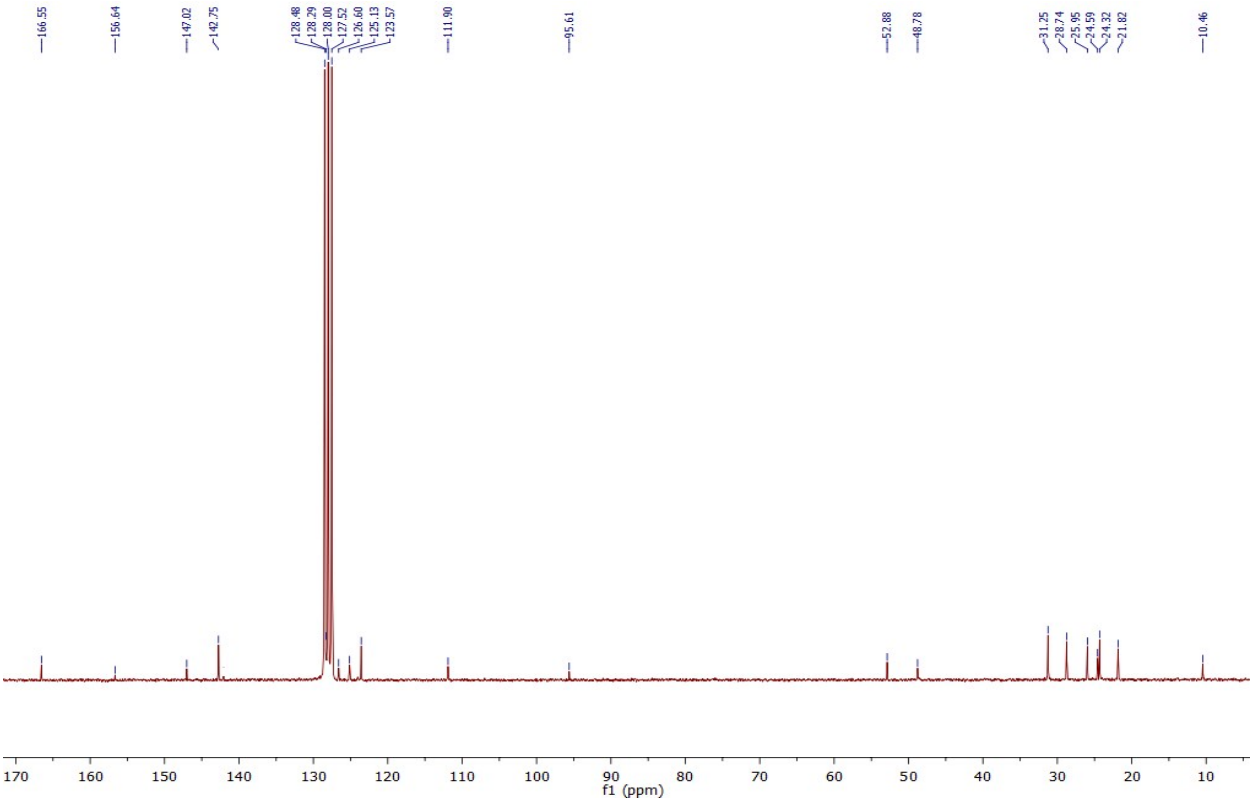

Figure S8. ^{13}C{^{1}H}-NMR spectrum of **5** in C_6D_6 at 298 K.

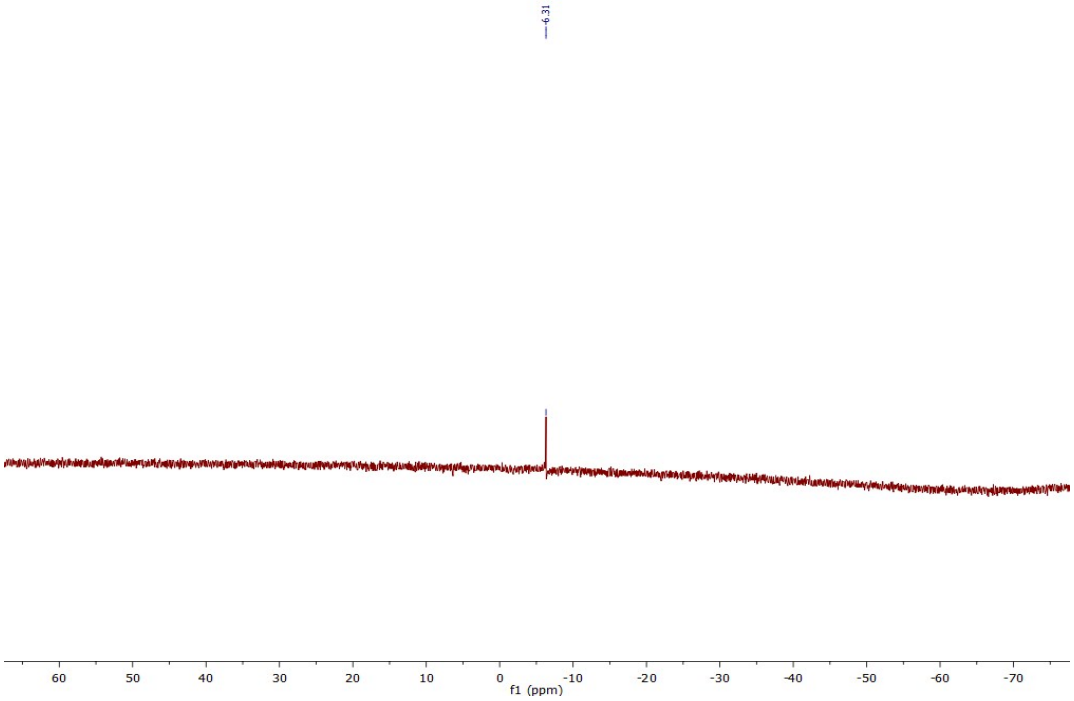

Figure S9. $^{29}Si\{^{1}H\}$-NMR spectrum of **5** in C_6D_6 at 298 K.

1.1.4. Synthesis of [{(*t*BuNHSi)→AsZnL}$_2$] (6)

A Et_2O (25 mL) solution of **1** (0.36 g, 0.71 mmol) at ambient temperature was added dropwise to a suspension of NaAsCO(dioxane)$_{2,3}$ (0.25 g, 0.78 mmol, 1.1 eq.) in Et_2O (15 mL) precooled at 0 °C. The white mixture was stirred and warmed up to ambient temperature in 30 minutes, after this, a blue solution mixed with a colorless to red solid was obtained. The sensitive and blue solution containing LZnAsCO was Teflon-cannula filtered and immediately added to a Et_2O (15 mL) solution of *t*BuNHSi (0.14 g, 0.71 mmol) at ambient temperature under stirring. The resulting solution became green, gas evolution was observed, and after one hour, a fine and yellow solid precipitated from the mixture. Then, the solution was filtered, the solid was washed with Et_2O (2 x 5 mL) and hexane (2 x 2 mL) and dried under vacuum. Yield: 0.16 g (30 %), m.p. 226 °C (d.). Crystals of **6** can be obtained from a saturated THF solution of the crude solid. Elemental analysis calcd (%) for $C_{78}H_{122}N_8As_2Si_2Zn_2$: C 62.10, H 8.15, N 7.43; found: C 62.05, H 8.24, N 7.15. ^{1}H NMR (C_6D_6, 200 MHz, 298 K): δ (ppm) = 1.13 (d, $^{3}J_{HH}$ = 6.8 Hz, 12H, L-*i*Pr-C*H*$_3$), 1.36 (s, 18H, NHSi-*t*Bu-C*H*$_3$), 1.37 (d, $^{3}J_{HH}$ = 6.8 Hz, 12H, L-*i*Pr-C*H*$_3$), 1.45 (s, 6H, L-NC*Me*), 3.12 (sept, $^{3}J_{HH}$ = 6.8 Hz, 4H, L-*i*Pr-C*H*), 4.93 (s, 1H, L-NCC*H*CN), 5.67 (s, 2H, NHSi-NC*H*), 7.11 (s, 6 H; *m* and *p* -Ar*H*). CP/MAS $^{29}Si\{^{1}H\}$-NMR δ (ppm) = -23.53.

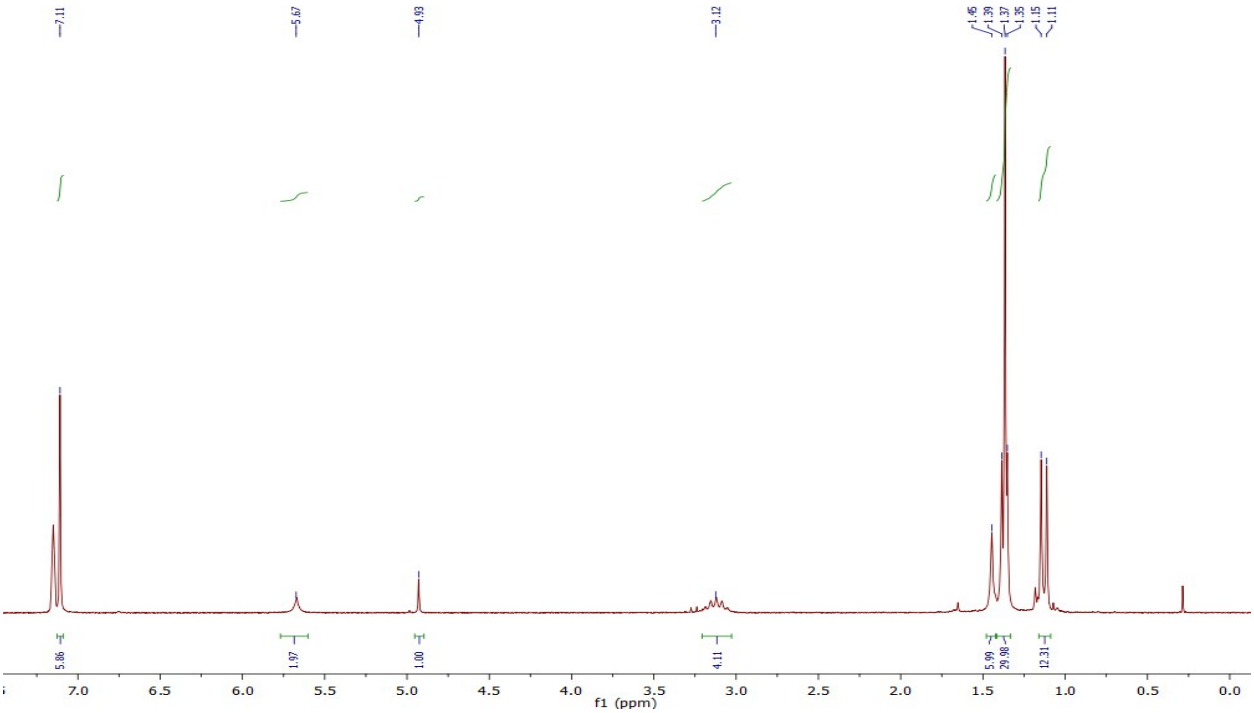

Figure S10. ^{1}H-NMR spectrum of **6** in C_6D_6 at 298 K.

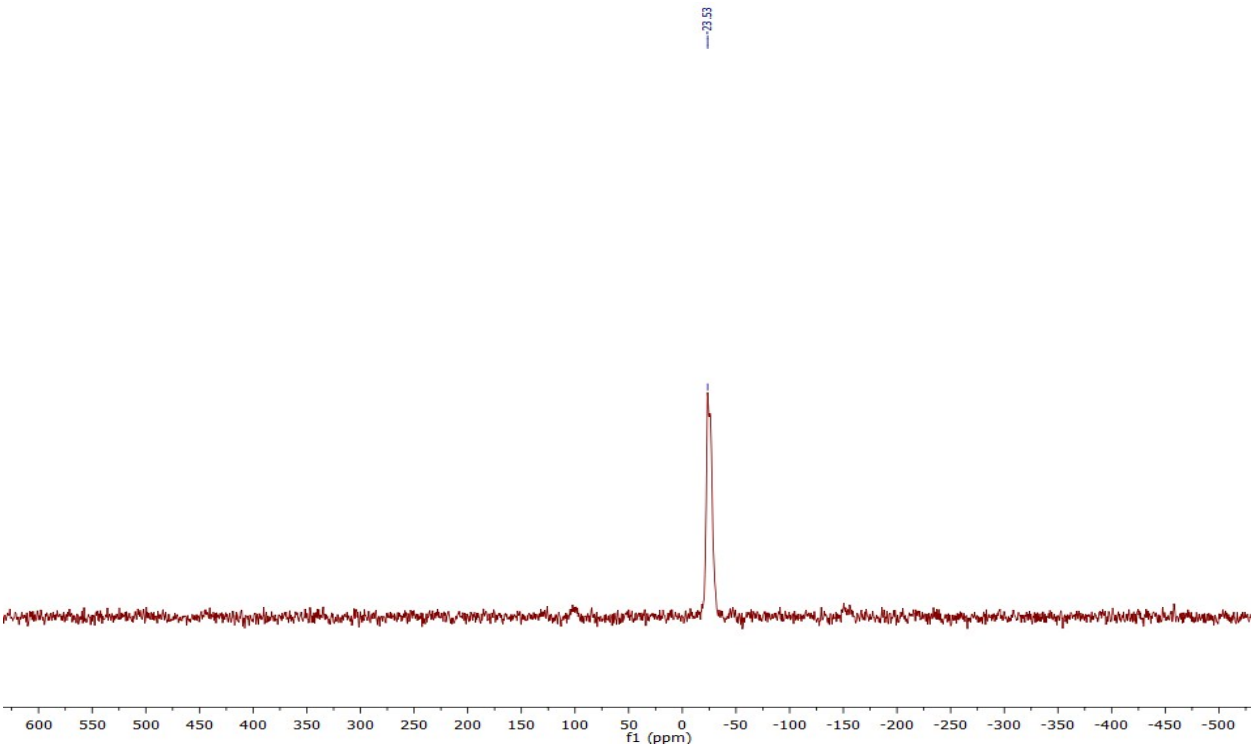

Figure S11. CP/MAS ^{29}Si-NMR spectrum of **6** in C_6D_6 at 298 K.

1.1.5. Synthesis of [(DippNHSi)→AsZnL] (7)

A Et_2O (50 mL) solution of **1** (0.81 g, 1,1 mmol) at ambient temperature was added dropwise to a suspension of NaAsCO(dioxane)$_{2,3}$ (0.43 g, 1.3 mmol, 1.1 eq.) in Et_2O (20 mL) precooled at 0 °C. The white mixture was stirred and warmed up to ambient temperature in 40 minutes, after this, a blue solution mixed with a colorless to red solid was obtained. The sensitive and blue solution containing LZnAsCO was Teflon-cannula filtered and immediately added to a Et_2O (10 mL) solution of DippNHSi (0.38 g, 1.1 mmol) at ambient temperature under stirring. The resulting solution became darker, gas evolution was observed, and after one hour, the volatiles were removed under vacuum. The mixture was extracted with hexane (20 mL) and the volume of the solution was reduced until the incipient formation of orange crystals. The mixture was kept at ambient temperature overnight. After this, a first batch of **7** was collected, washed with hexane (2 mL), and dried under vacuum. Given the high solubility of **7** in hexane, one additional crystallization from the mother liquor were carried out at 4 °C. Yield: 0.20 g (19 %), m.p. 193 °C (d.). Elemental analysis calcd (%) for $C_{55}H_{77}N_4AsSiZn$: C 68.62, H 8.06, N 5.82; found: C 69.12, H 8.24, N 5.61. ^{1}H NMR (C_6D_6, 200 MHz, 298 K): δ (ppm) = 1.05-1.22 (m, 48H, L- and NHSi- ^{i}Pr-C*H*$_3$), 1.54 (s, 6H, L-NC*Me*), 3.15 and 3.28 (2 x sept, $^3J_{HH}$ = 6.9 Hz, 8H, L- and DippNHSi- ^{i}Pr-C*H*), 4.89 (s, 1H, L -NCC*H*CN), 5.85 (s, 2H, NHSi-NC*H*), 7.00-7.14 (m, 12H; L and DippNHSi *m* and *p* Ar*H*). ^{13}C{^{1}H}-NMR (C_6D_6, 50 MHz, 298 K): δ (ppm) = 24.40 (L-C*Me*), 24.01, 24.81, 25.09 and 25.17 (L- and NHSi- ^{i}Pr-*C*H$_3$), 28.61 and 28.84 (L- and NHSi- ^{i}Pr-*C*H), 96.94 (L -NC*C*HCN), 122.93 (NHSi -N*C*H), 123.94, 124.09, 126.22 and 128.28 (L and DippNHSi *m* and *p* -Ar*C*), 138.15 and 142.61 (L and DippNHSi *o*-Ar*C*), 144.84 and 146.07 (L and DippNHSi *i*-Ar*C*), 168.04 (L-NCC*H*CN). ^{29}Si{^{1}H}-NMR (C_6D_6, 79 MHz, 298 K) δ (ppm) = 65.86.

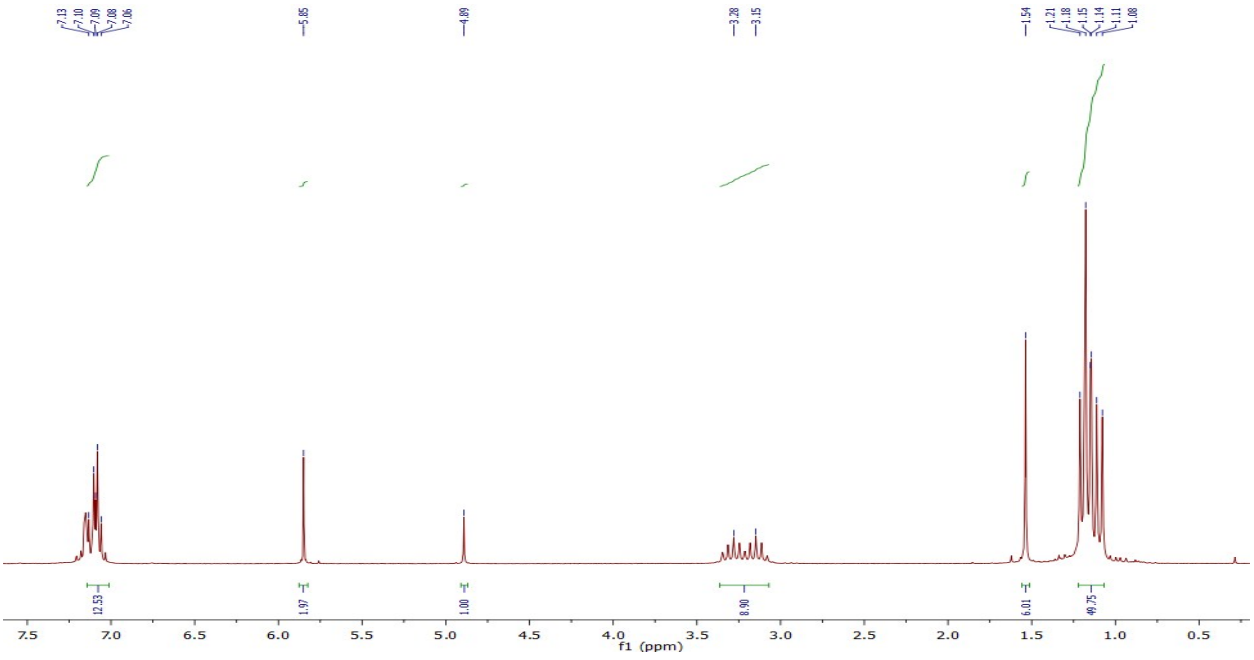

Figure S12. ^{1}H-NMR spectrum of **7** in C_6D_6 at 298 K.

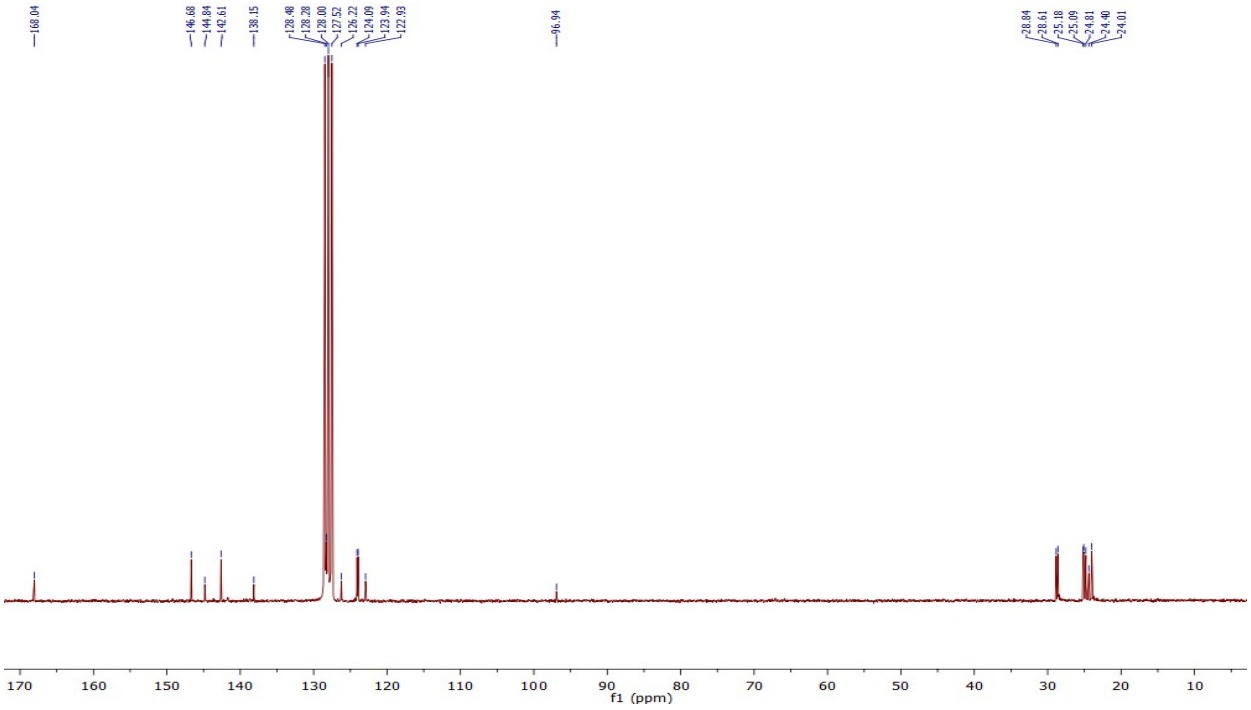

Figure S13. $^{13}C\{^{1}H\}$-NMR spectrum of **7** in C_6D_6 at 298 K.

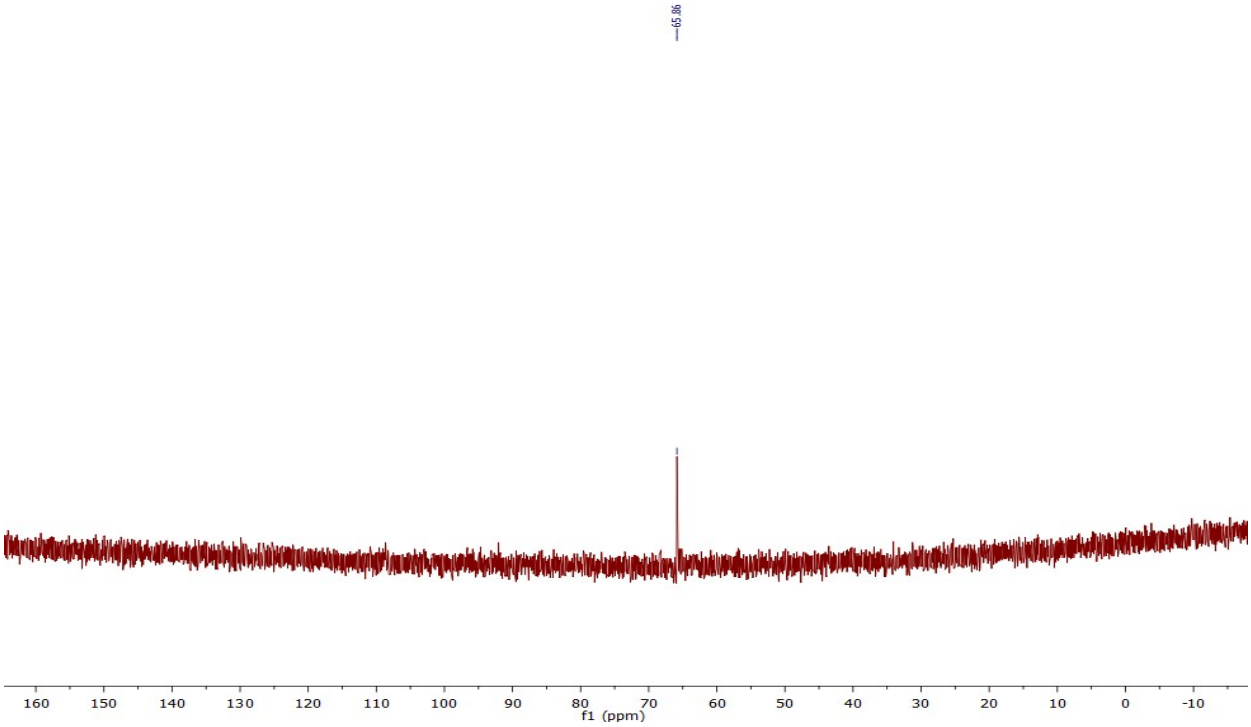

Figure S14. $^{29}Si\{^{1}H\}$-NMR spectrum of **7** in C_6D_6 at 298 K.

2. Crystallographic data

Crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data of compounds **3**-**7** were collected on an Oxford Diffraction Supernova, Single source at offset, Atlas at 150 K (Cu-Kα-radiation, λ = 1.54184 Å). The structures were solved by direct methods or using the SHELXT program[6] and refined on F2 with the SHELX-2016 software package.[7] The positions of the H atoms were calculated and considered isotropically according to a riding model. CCDC 1828201 (**3**), 1828202 (**4**), 1828203 (**5**), 1828204 (**6**) and 1828205 (**7**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge by contacting The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

Table S1. Summary of Crystallographic Data for Compounds **3**-**7**.

	3	**4**	**5**	**6**	**7**
CCDC	1828201	1828202	1828203	1828204	1828205
empirical form.	$C_{40}H_{61}ClN_4Zn$	$C_{41}H_{61}AsN_4OZn$	$C_{50}H_{81}AsN_6SiZn$	$C_{39}H_{61}AsN_4SiZn$	$C_{55}H_{77}AsN_4SiZn$
formula wt	698.74	766.22	934.68	754.29	962.58
crystal syst.	orthorhombic	monoclinic	triclinic	monoclinic	monoclinic
space group	*P 2₁ 2₁ 2₁*	*P 2₁/n*	*P-1*	*P 2₁/c*	*P 2₁/c*
a (Å)	11.83520(10)	17.2926(2)	13.5770(6)	13.8602(2)	14.0308(1)
b (Å)	17.5939(2)	11.8957(1)	14.7552(5)	21.5672(3)	13.9065(1)
c (Å)	18.3290(2)	19.9787(2)	14.8121(5)	12.9197(1)	26.7370(2)
α (deg)	90	90	92.378(3)	90	90
β (deg)	90	104.184(1)	107.476(4)	95.682(1)	90.031(1)
γ (deg)	90	90	112.237(4)	90	90
vol (Å^3)	3816.60(7)	3984.48(7)	2579.10(19)	3843.06(8)	5216.90(7)
Z	4	4	2	4	4
ρ_{calcd} (g/cm^3)	1.216	1.277	1.203	1.304	1.226
μ (mm^{-1})	1.767	2.038	1.872	2.372	1.858
F(000)	1504	1624	1000	1600	2048
reflns collect.	15746	15940	18017	14765	25494
unique reflns	6952	7530	9688	7231	10200
R_{int}	0.0388	0.0240	0.0417	0.0218	0.0289
R1 [I>2σ(I)]	0.0370	0.0407	0.0411	0.0284	0.0372
wR2	0.0988	0.01192	0.1201	0.0826	0.1018

2.1. Molecular structure of LZnCl(NHC) (3)

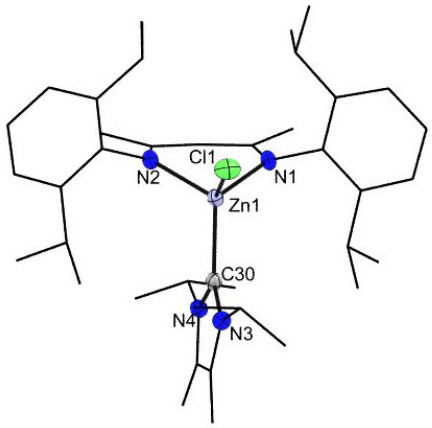

Figure S15. Molecular structure of **3**. Thermal ellipsoids are drawn at 50 % probability. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°] for **3**: N1-Zn1 2.038(2), N2-Zn1: 2.038(2), Zn1-Cl1 2.254(1), Zn1-Zn30 2.097(2), N1-Zn1-N2 94.13(8), C30-Zn1-C11 115.13(7).

3. Computational data

Computational details:

DFT calculations were performed at the B3LYP-D3/def2-SVP[Si,Ni,As:def2-TZVP] level of theory.[8-11] Stationary points on the potential energy surface (PES) were characterized by harmonic vibrational frequency calculations. Electronic structure analysis and NMR shift calculations were executed at the same B3LYP-D3/def2-SVP[Si,Ni,As:def2-TZVP] level of theory. Calculations were carried out using the GAUSSIAN 09 program suite.[12]

3.1. Compound [NHC→^{t}BuNHSi→AsZnL] (5)

NPA charge: Si: +1.61; As: -1.03; Zn: +0.99
MBO: Si1-As1: 1.31; Zn1-As1: 1.02
WBI: Si1-As1: 1.33; Zn1-As1: 0.87
Natural Ionicity: Si1-As1: 0.24; Zn1-As1: 0.77
^{29}Si-NMR: -1 ppm

Table S3. NBO analysis of compound **5**.

NBO	atom	Occupation	polarization	s-character	p-character	d-character
Bond	Si	1.94	44.00%	46.49%	52.94%	0.54%
	As		56.00%	18.64%	80.61%	0.71%
Bond	Zn	1.90	26.27%	92.29%	6.58%	1.13%
	As		73.73%	10.17%	89.11%	0.72%
Lone pair	As	1.84	-	71.15%	28.70%	0.14%
Lone pair	As	1.61	-	0.00%	99.64%	0.33%

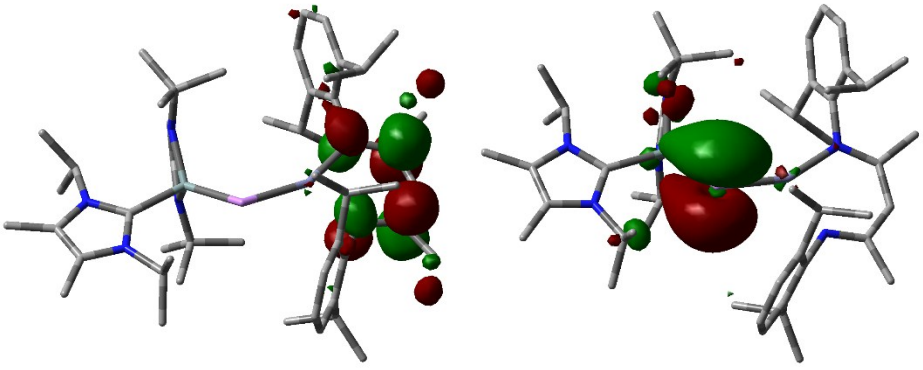

Figure S16. LUMO (left, -1.31 eV) and HOMO (right, -2.91 eV) of **5**. Isovalues are 0.04 au.

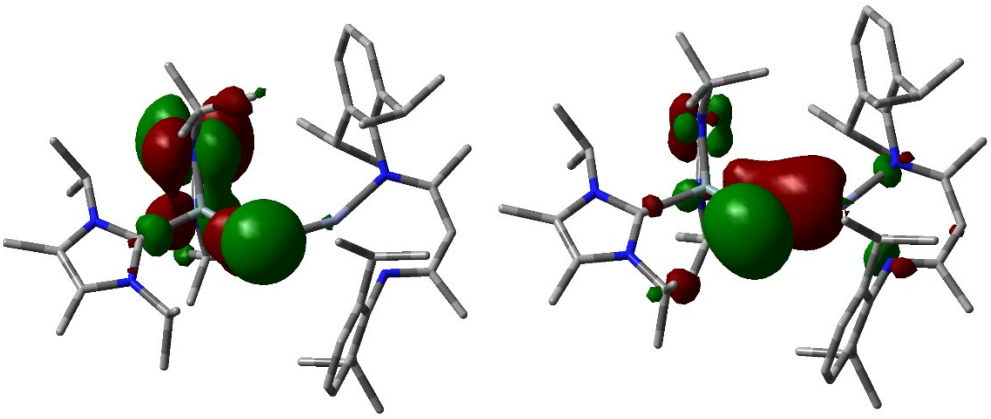

Figure S17. HOMO-1 (left, -3.02 eV) and HOMO-2 (right, -4.09 eV) of **5**. Isovalues are 0.04 au.

3.2. Compound [{(ᵗBuNHSi)→AsZnL}$_2$] (6)

NPA charge: Si: +1.55; As: -0.95; Zn: +1.14
MBO: As1-Si1: 1.07; As1- Si1': 0.80; Zn1-As1: 0.89
WBI: As1-Si1: 1.03; As1- Si1': 0.78; Zn1-As1: 0.65
Natural Ionicity: As1-Si1: 0.40; As1- Si1' 0.61; Zn1-As1: 0.89
^{29}Si-NMR: -15 ppm

Table S4. NBO analysis of compound **6**.

NBO	atom	Occupation	polarization	s-character	p-character	d-character
Bond	Si	1.92	33.08%	32.04%	66.74%	1.20%
	As		66.92%	20.82%	78.74%	0.40%
Bond	Si	1.94	39.66%	39.64%	59.39%	0.94%
	As		60.34%	19.30%	80.10%	0.56%
Bond	Zn	1.94	19.30%	86.63%	12.60%	0.77%
	As		80.70%	17.79%	81.93%	0.26%
Lone pair	As	1.78	-	41.91%	57.93%	0.15%

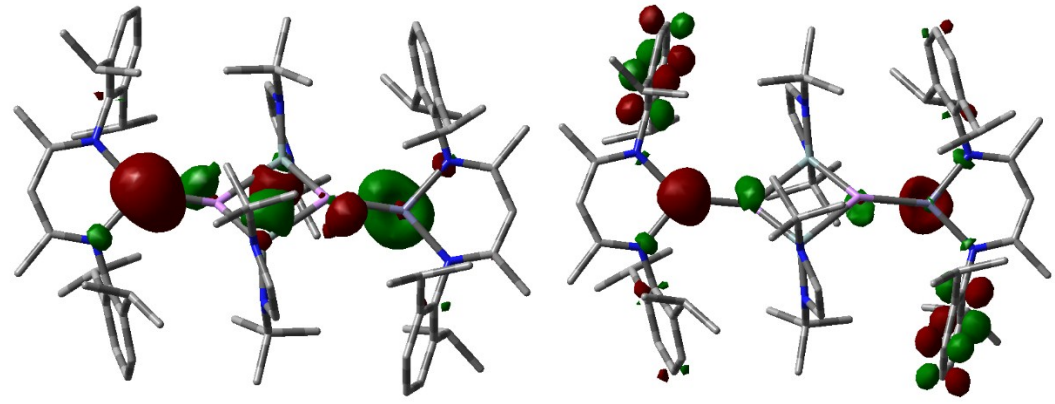

Figure S18. LUMO+2 (left, -0.59 eV) and LUMO+3 (right, -0.32 eV) of **6**. Isovalues are 0.04 au.

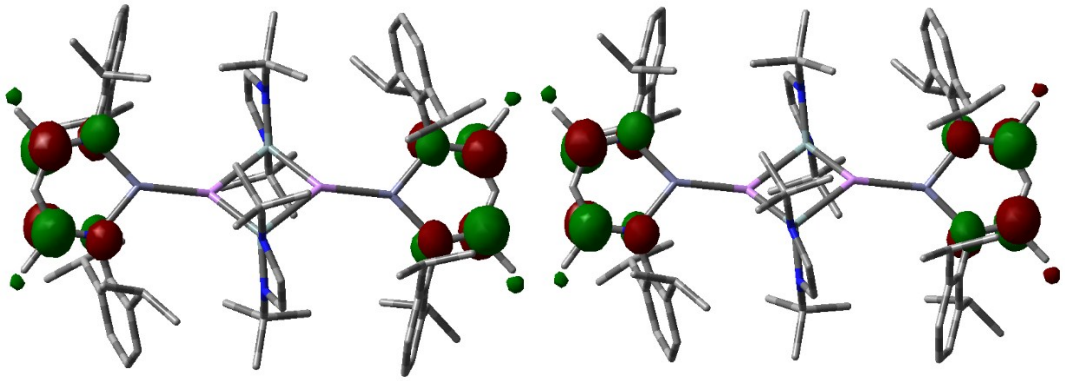

Figure S19. LUMO (left, -1.11 eV) and LUMO+1 (right, -1.11 eV) of **6**. Isovalues are 0.04 au.

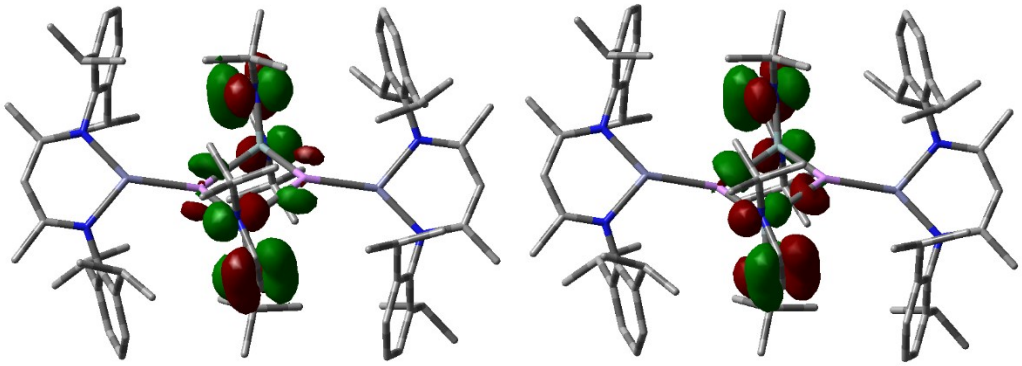

Figure S20. HOMO (left, -3.86 eV) and HOMO-1 (right, -4.16 eV) of **6**. Isovalues are 0.04 au.

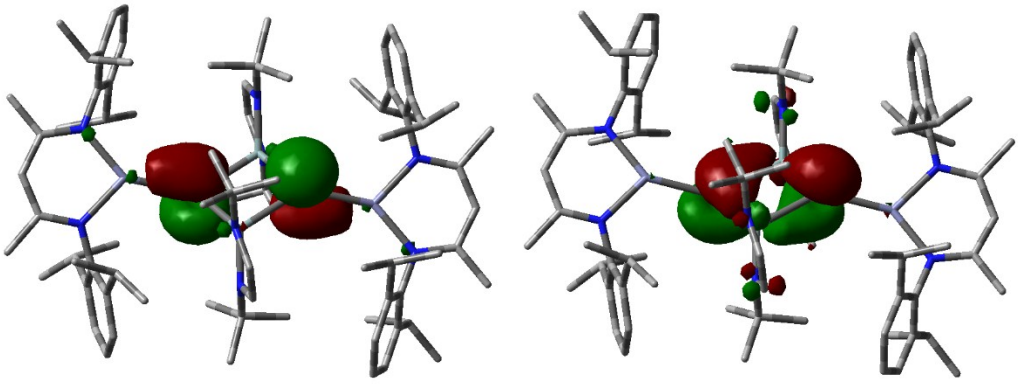

Figure S21. HOMO-2 (left, -4.48 eV) and HOMO-3 (right, -5.02 eV) of **6**. Isovalues are 0.04 au.

3.3. Compound [(DippNHSi)→AsZnL] (7)

NPA charge: Si: +1.41; As: -0.82; Zn: +1.05
MBO: Si1-As1: 1.66; Zn1-As1: 0.95
WBI: Si1-As1: 1.72; Zn1-As1: 0.77
Natural Ionicity: Si1-As1(σ): 0.00; Si1-As1(π_1): 0.88; Si1-As1(π_2): 0.93
^{29}Si-NMR: +74 ppm

Table S5. NBO analysis of compound **7**. Orbital number is in parenthesis.

NBO	atom	Occupation	polarization	s-character	p-character	d-character
Bond (NBO-152)	Si	1.96	49.98%	70.42%	29.28%	0.26%
	As		50.02%	12.33%	86.71%	0.91%
Bond (NBO-256)	Si	1.91	19.81%	0.16%	98.23%	1.45%
	As		80.19%	0.38%	98.88%	0.70%
Bond (NBO-244)	Si	1.62	16.15%	0.06%	98.54%	1.28%
	As		83.85%	5.53%	93.13%	1.32%
Anti-bond (NBO-260)	Si	0.32	16.15%	0.06%	98.54%	1.28%
	As		83.85%	5.53%	93.13%	1.32%
Lone pair (NBO-123)	As	1.82	-	81.83%	18.06%	0.11%
Empty lone pair (NBO-257)	Zn	0.57	-	98.11%	1.10%	0.80%

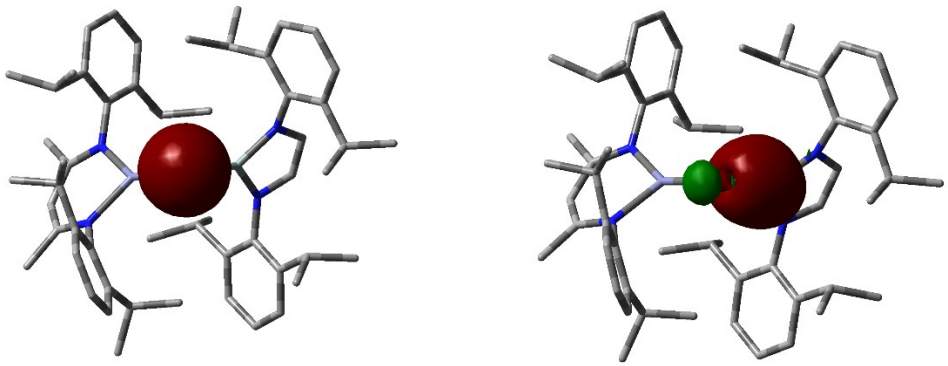

Figure S22. NBO-123 (left) and NBO-152 (right) of **7**. Isovalues are 0.04 au.

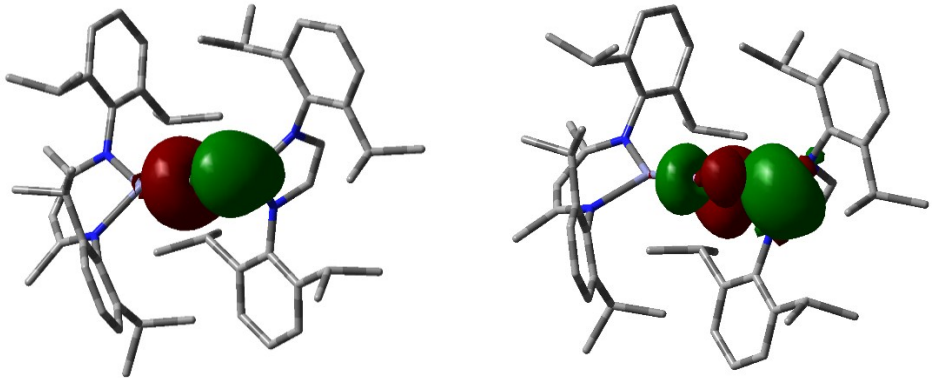

Figure S23. NBO-244 (left) and NBO-260 (right) of **7**. Isovalues are 0.04 au.

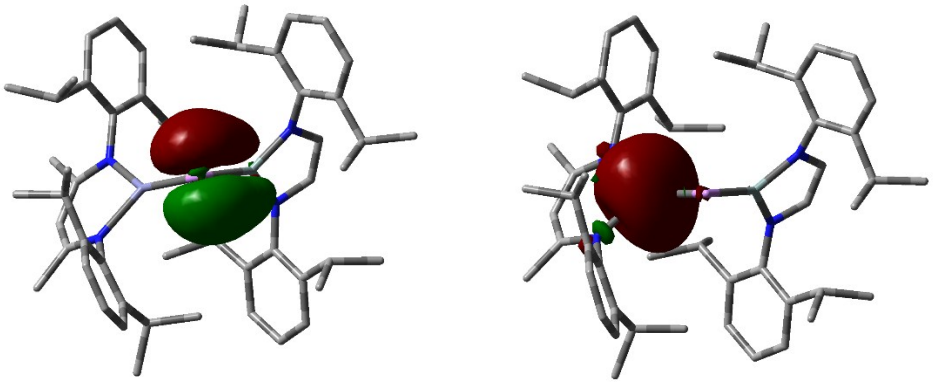

Figure S24. NBO-256 (left) and NBO-257 (right) of **7**. Isovalues are 0.04 au.

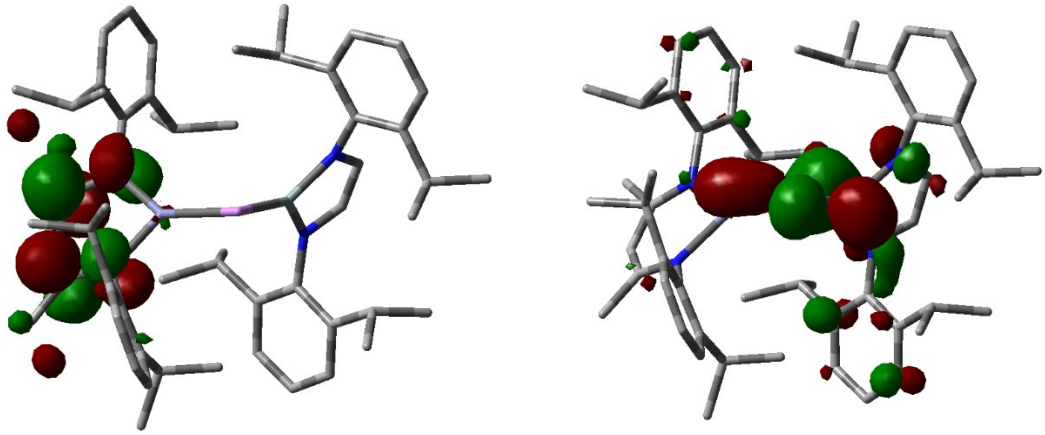

Figure S25. LUMO (left, -1.14 eV) and LUMO+1 (right, -0.68 eV) of **7**. Isovalues are 0.04 au.

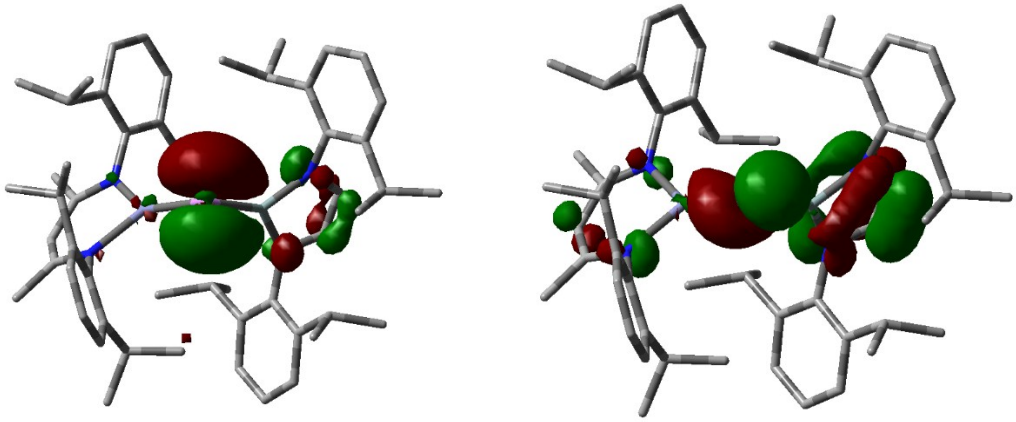

Figure S26. HOMO (left, -4.57 eV) and HOMO-1 (right, -5.38 eV) of **7**. Isovalues are 0.04 au.

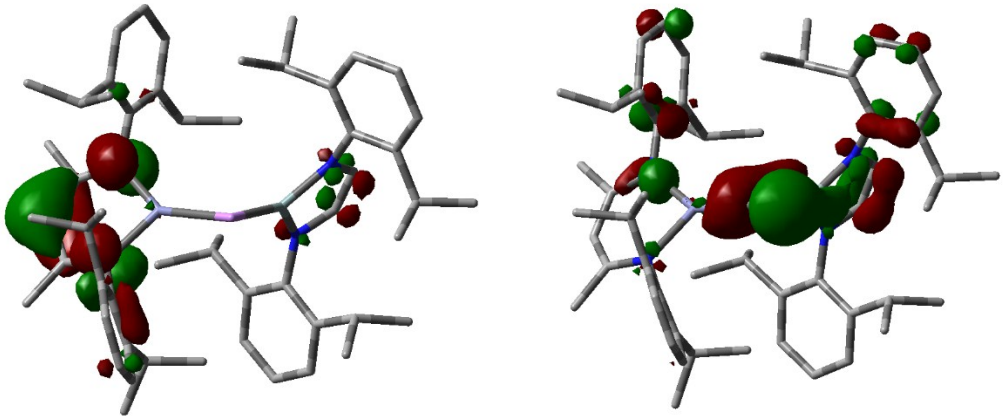

Figure S27. HOMO-2 (left, -5.62 eV) and HOMO-4 (right, -6.32 eV) of **7**. Isovalues are 0.04 au.

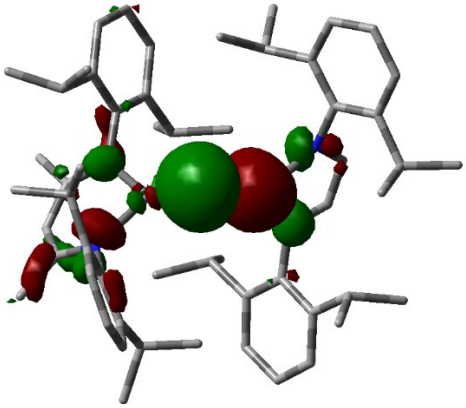

Figure S28. HOMO-12 (-7.59 eV) of **7**. Isovalues are 0.04 au.

3.4. Optimized geometries for compounds 5-7.

Table S6. Cartesian geometry of **5** in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
As	-0.329564	0.832956	-0.643332
Zn	1.714323	0.106757	0.2144
Si	-1.945385	-0.570064	0.047966
C	-3.722702	0.286192	-0.432368
N	3.184829	-1.199035	0.535957
N	-4.027087	1.593243	-0.686416
N	-2.01265	-2.249183	-0.526155
N	2.948988	1.759994	0.404276
N	-2.260689	-1.101927	1.721853
N	-4.915954	-0.377569	-0.479091
C	-0.138951	-2.99459	-1.96124

H	0.392021	-2.048598	-1.798313
H	0.149721	-3.398892	-2.944989
H	0.194817	-3.702125	-1.188869
C	-2.104792	-1.748405	-2.933794
H	-3.192422	-1.57856	-2.880476
H	-1.86478	-2.124206	-3.940512
H	-1.593853	-0.784257	-2.797907
C	1.737932	-2.973441	2.344822
H	1.182305	-2.045171	2.120842
C	3.388871	-2.958295	-1.15595
C	2.962458	-2.551771	0.132867
C	5.466137	-1.927654	1.111716
H	5.063072	-2.80726	1.631217
H	6.333973	-1.547967	1.666645
H	5.816249	-2.279107	0.128372
C	4.016039	-1.963944	-2.130822
H	4.406831	-1.11749	-1.549634
C	-3.043157	2.704468	-0.722525
H	-2.112737	2.248938	-0.349838
C	2.333735	3.281738	-1.404853
C	2.389747	3.00314	-0.014807
C	2.819333	-2.62286	3.384531
H	3.466841	-3.493251	3.583145
H	2.344162	-2.336201	4.337107
H	3.451169	-1.783481	3.072077
C	4.191615	1.692055	0.856837
C	-1.657097	-2.766332	-1.870078
C	4.416142	-0.845162	0.934637
C	-2.177496	-2.504881	1.778519
H	-2.234897	-3.030724	2.727845
C	-2.034435	-3.1185	0.584652
H	-1.967946	-4.195981	0.4563
C	2.294983	-3.450373	1.002636
C	2.125814	-4.775656	0.574029
H	1.628767	-5.496768	1.222757
C	4.846041	0.473379	1.162586
H	5.864665	0.572104	1.535346
C	-2.158339	-0.299382	2.961726
C	2.57031	-5.197403	-0.679124
H	2.422235	-6.234827	-0.990149
C	1.807237	3.888509	0.921465
C	-2.695081	1.113874	2.680855
H	-2.128621	1.595508	1.873363

H	-2.601641	1.746043	3.576766
H	-3.757127	1.075153	2.391408
C	-5.392147	1.743085	-0.903242
C	3.179844	-4.288914	-1.541239
H	3.49612	-4.62041	-2.532506
C	0.748433	-3.961326	2.974173
H	-0.046069	-4.243612	2.271822
H	0.268093	-3.503568	3.8532
H	1.259483	-4.874291	3.322784
C	-5.955507	0.501144	-0.766573
C	5.196958	-2.548105	-2.91981
H	5.946924	-3.001706	-2.252048
H	5.693356	-1.755686	-3.502926
H	4.875116	-3.322304	-3.635122
C	2.950502	-1.389652	-3.079834
H	2.48812	-2.188129	-3.68219
H	3.400099	-0.655191	-3.766779
H	2.145456	-0.885225	-2.523949
C	4.987233	2.966322	1.065765
H	4.898811	3.636712	0.198917
H	6.048479	2.755847	1.251391
H	4.587386	3.520631	1.928686
C	-0.69124	-0.225767	3.43448
H	-0.319425	-1.233989	3.667999
H	-0.591133	0.395876	4.338555
H	-0.057031	0.198972	2.643555
C	-5.082572	-1.810867	-0.129737
H	-4.062717	-2.196787	-0.110033
C	-2.389221	-4.095666	-2.14705
H	-2.032288	-4.912475	-1.502604
H	-2.209603	-4.406163	-3.187867
H	-3.474644	-3.989374	-2.002451
C	1.712893	3.543614	2.402858
H	2.306218	2.633469	2.574028
C	-6.080146	3.034648	-1.210941
H	-5.53204	3.623702	-1.957537
H	-6.198459	3.662847	-0.314014
H	-7.081565	2.838593	-1.616051
C	2.887422	2.28852	-2.421525
H	2.810591	1.291444	-1.964702
C	1.749137	4.48342	-1.823695
H	1.706052	4.718662	-2.888597
C	-5.825977	-2.60911	-1.203276

H	-6.912699	-2.450649	-1.196231
H	-5.653778	-3.680034	-1.017984
H	-5.440637	-2.378032	-2.207529
C	-3.01145	-0.910561	4.091777
H	-4.057776	-1.040236	3.776889
H	-2.997647	-0.242389	4.966671
H	-2.630109	-1.886825	4.425178
C	1.227072	5.075824	0.452918
H	0.773942	5.76773	1.167521
C	-5.67388	-1.96797	1.270358
H	-5.077601	-1.394099	1.990938
H	-5.625516	-3.026932	1.564234
H	-6.72411	-1.642684	1.332667
C	0.255605	3.20652	2.759222
H	-0.389759	4.095983	2.662375
H	0.172347	2.836811	3.794311
H	-0.128775	2.437775	2.074313
C	-3.380682	3.848309	0.235279
H	-4.116776	4.561479	-0.163403
H	-2.452222	4.40799	0.428461
H	-3.744236	3.465567	1.20052
C	-7.395832	0.128748	-0.91876
H	-8.015818	1.034599	-0.91596
H	-7.748935	-0.511366	-0.099148
H	-7.587531	-0.404063	-1.863605
C	2.268855	4.644868	3.319298
H	3.308383	4.905619	3.065078
H	2.246744	4.318178	4.371962
H	1.671512	5.568535	3.250677
C	2.073541	2.240711	-3.720327
H	1.007488	2.073555	-3.502924
H	2.425331	1.414337	-4.357516
H	2.173789	3.167404	-4.308892
C	1.205644	5.382921	-0.90584
H	0.754803	6.316664	-1.252777
C	4.379488	2.531748	-2.705855
H	4.540089	3.536273	-3.131996
H	4.763441	1.790599	-3.426849
H	4.98479	2.450234	-1.791195
C	-2.736646	3.156629	-2.1483
H	-2.469645	2.292837	-2.773953
H	-1.859014	3.820805	-2.120963
H	-3.569021	3.702797	-2.620097

Table S7. Cartesian geometry of **6** in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
Zn	-3.235346	0.611532	-2.175306
As	-1.107024	0.000512	-1.299721
Si	0.998252	1.071167	-0.742326
N	-4.589061	-0.742313	-2.768733
N	1.131728	2.820993	-0.840429
N	-4.065519	2.186391	-3.119695
N	2.148103	0.863359	-2.064428
C	-3.317555	3.40058	-3.237425
C	0.51639	3.890047	-0.014725
C	-3.699037	4.551167	-2.505528
C	-1.807718	2.184377	-4.923976
H	-1.898259	1.313209	-4.252924
C	-5.235026	2.083858	-3.761121
C	-1.689856	-1.743102	-4.849942
H	-1.461305	-1.225275	-3.906968
H	-1.325056	-1.122875	-5.685339
H	-1.122515	-2.688209	-4.850367
C	-5.799185	3.271061	-4.521941
H	-6.437964	3.875231	-3.858766
H	-6.42046	2.92848	-5.359944
H	-5.010259	3.928101	-4.907079
C	-0.962262	4.032908	-0.390035
H	-1.059129	4.267002	-1.45658
H	-1.44482	4.835116	0.187756
H	-1.501848	3.094481	-0.210135
C	-4.299651	-2.139889	-2.66448
C	-2.202913	3.422479	-4.116843
C	2.183265	2.081029	-2.771259
H	2.643059	2.144913	-3.755106
C	-2.963829	5.730658	-2.689177
H	-3.240228	6.627936	-2.130029
C	1.62791	3.126843	-2.12131
H	1.572019	4.135503	-2.521682
C	-1.4957	4.625074	-4.255366
H	-0.634075	4.671036	-4.922768
C	2.692407	-0.345397	-2.723055
C	4.154882	-0.099398	-3.141539
H	4.250632	0.720085	-3.868735

H	4.568357	-1.006986	-3.608394
H	4.766372	0.147392	-2.260689
C	-4.87217	4.540427	-1.527696
H	-5.457567	3.630067	-1.712159
C	-6.017734	0.914728	-3.82447
H	-6.951571	1.016853	-4.376606
C	-3.199024	-2.01053	-4.97677
H	-3.696771	-1.030478	-4.973623
C	-5.686229	-0.400981	-3.451282
C	0.668333	3.558346	1.476112
H	0.120709	2.650854	1.753682
H	0.279598	4.388922	2.085625
H	1.723531	3.39978	1.731776
C	-6.621031	-1.486323	-3.947869
H	-6.155756	-2.022252	-4.789133
H	-7.571747	-1.060595	-4.293595
H	-6.819347	-2.239076	-3.173478
C	-3.694765	-2.793608	-3.7641
C	-4.650353	-2.842425	-1.486873
C	-4.389038	4.456921	-0.07138
H	-3.76971	3.565498	0.090454
H	-5.247491	4.409612	0.618872
H	-3.785017	5.338799	0.195675
C	-3.516236	-4.181844	-3.697572
H	-3.04935	-4.706552	-4.534608
C	-4.467601	-4.233316	-1.477963
H	-4.74513	-4.807815	-0.59357
C	-3.922865	-4.902188	-2.575213
H	-3.783434	-5.98601	-2.538751
C	-1.875974	5.774248	-3.559193
H	-1.31134	6.701951	-3.686284
C	2.685092	-1.522419	-1.745872
H	3.279028	-1.295616	-0.84816
H	3.103079	-2.416638	-2.231243
H	1.668425	-1.75978	-1.415361
C	-2.747875	1.935601	-6.117456
H	-3.789999	1.788399	-5.807842
H	-2.435282	1.030746	-6.663925
H	-2.711861	2.784912	-6.819567
C	1.232152	5.232005	-0.26589
H	2.317917	5.124406	-0.133583
H	0.869809	5.977773	0.457684
H	1.029817	5.632136	-1.270278

C	-5.811865	5.742289	-1.715124
H	-5.330471	6.684168	-1.405858
H	-6.716239	5.621154	-1.097158
H	-6.123756	5.858553	-2.764462
C	1.843961	-0.708576	-3.957943
H	0.803691	-0.894502	-3.657547
H	2.23534	-1.612511	-4.451529
H	1.843907	0.110416	-4.693094
C	-0.353674	2.197543	-5.40431
H	-0.190184	2.952164	-6.191362
H	-0.097559	1.217143	-5.835408
H	0.339111	2.395251	-4.57433
C	-5.18594	-2.107664	-0.255624
H	-4.550769	-1.211405	-0.134509
C	-6.640937	-1.626034	-0.404806
H	-6.757499	-0.870902	-1.192018
H	-6.982797	-1.171924	0.539733
H	-7.310721	-2.473093	-0.628542
C	-3.531053	-2.681806	-6.316786
H	-2.972129	-3.621753	-6.453633
H	-3.258648	-2.016781	-7.152241
H	-4.604704	-2.914385	-6.401101
C	-5.057409	-2.932937	1.027547
H	-5.762771	-3.780882	1.03126
H	-5.296512	-2.310764	1.902046
H	-4.039306	-3.316304	1.166954
As	1.107024	-0.000512	1.299721
Si	-0.998252	-1.071167	0.742326
N	-1.131728	-2.820993	0.840429
N	-2.148103	-0.863359	2.064428
C	-0.51639	-3.890047	0.014725
C	0.962262	-4.032908	0.390035
H	1.059129	-4.267002	1.45658
H	1.44482	-4.835116	-0.187756
H	1.501848	-3.094481	0.210135
C	-2.183265	-2.081029	2.771259
H	-2.643059	-2.144913	3.755106
C	-1.62791	-3.126843	2.12131
H	-1.572019	-4.135503	2.521682
C	-2.692407	0.345397	2.723055
C	-4.154882	0.099398	3.141539
H	-4.250632	-0.720085	3.868735
H	-4.568357	1.006986	3.608394

H	-4.766372	-0.147392	2.260689
C	-0.668333	-3.558346	-1.476112
H	-0.120709	-2.650854	-1.753682
H	-0.279598	-4.388922	-2.085625
H	-1.723531	-3.39978	-1.731776
C	-2.685092	1.522419	1.745872
H	-3.279028	1.295616	0.84816
H	-3.103079	2.416638	2.231243
H	-1.668425	1.75978	1.415361
C	-1.232152	-5.232005	0.26589
H	-2.317917	-5.124406	0.133583
H	-0.869809	-5.977773	-0.457684
H	-1.029817	-5.632136	1.270278
C	-1.843961	0.708576	3.957943
H	-0.803691	0.894502	3.657547
H	-2.23534	1.612511	4.451529
H	-1.843907	-0.110416	4.693094
Zn	3.235346	-0.611532	2.175306
N	4.589061	0.742313	2.768733
N	4.065519	-2.186391	3.119695
C	3.317555	-3.40058	3.237425
C	3.699037	-4.551167	2.505528
C	1.807718	-2.184377	4.923976
H	1.898259	-1.313209	4.252924
C	5.235026	-2.083858	3.761121
C	1.689856	1.743102	4.849942
H	1.461305	1.225275	3.906968
H	1.325056	1.122875	5.685339
H	1.122515	2.688209	4.850367
C	5.799185	-3.271061	4.521941
H	6.437964	-3.875231	3.858766
H	6.42046	-2.92848	5.359944
H	5.010259	-3.928101	4.907079
C	4.299651	2.139889	2.66448
C	2.202913	-3.422479	4.116843
C	2.963829	-5.730658	2.689177
H	3.240228	-6.627936	2.130029
C	1.4957	-4.625074	4.255366
H	0.634075	-4.671036	4.922768
C	4.87217	-4.540427	1.527696
H	5.457567	-3.630067	1.712159
C	6.017734	-0.914728	3.82447
H	6.951571	-1.016853	4.376606

C	3.199024	2.01053	4.97677
H	3.696771	1.030478	4.973623
C	5.686229	0.400981	3.451282
C	6.621031	1.486323	3.947869
H	6.155756	2.022252	4.789133
H	7.571747	1.060595	4.293595
H	6.819347	2.239076	3.173478
C	3.694765	2.793608	3.7641
C	4.650353	2.842425	1.486873
C	4.389038	-4.456921	0.07138
H	3.76971	-3.565498	-0.090454
H	5.247491	-4.409612	-0.618872
H	3.785017	-5.338799	-0.195675
C	3.516236	4.181844	3.697572
H	3.04935	4.706552	4.534608
C	4.467601	4.233316	1.477963
H	4.74513	4.807815	0.59357
C	3.922865	4.902188	2.575213
H	3.783434	5.98601	2.538751
C	1.875974	-5.774248	3.559193
H	1.31134	-6.701951	3.686284
C	2.747875	-1.935601	6.117456
H	3.789999	-1.788399	5.807842
H	2.435282	-1.030746	6.663925
H	2.711861	-2.784912	6.819567
C	5.811865	-5.742289	1.715124
H	5.330471	-6.684168	1.405858
H	6.716239	-5.621154	1.097158
H	6.123756	-5.858553	2.764462
C	0.353674	-2.197543	5.40431
H	0.190184	-2.952164	6.191362
H	0.097559	-1.217143	5.835408
H	-0.339111	-2.395251	4.57433
C	5.18594	2.107664	0.255624
H	4.550769	1.211405	0.134509
C	6.640937	1.626034	0.404806
H	6.757499	0.870902	1.192018
H	6.982797	1.171924	-0.539733
H	7.310721	2.473093	0.628542
C	3.531053	2.681806	6.316786
H	2.972129	3.621753	6.453633
H	3.258648	2.016781	7.152241
H	4.604704	2.914385	6.401101

C	5.057409	2.932937	-1.027547
H	5.762771	3.780882	-1.03126
H	5.296512	2.310764	-1.902046
H	4.039306	3.316304	-1.166954

Table S8. Cartesian geometry of **7** in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
As	-0.358526	-0.219692	-1.677071
Zn	1.4439	0.057121	-0.131666
Si	-1.851806	-0.093752	-0.10569
N	2.319138	1.320431	1.151881
C	4.059015	1.931554	2.781222
H	4.364462	2.868781	2.291858
H	4.935268	1.494853	3.276215
H	3.319395	2.209846	3.544609
N	3.020927	-1.184266	-0.35576
C	3.458985	0.972297	1.772006
N	-3.265866	0.912361	0.026384
C	4.183748	-0.208865	1.532973
H	5.058493	-0.348099	2.166123
N	-2.310581	-0.967855	1.334642
C	4.045834	-1.156983	0.489639
C	5.164804	-2.167556	0.338763
H	4.794324	-3.184768	0.531738
H	5.992782	-1.958593	1.027678
H	5.548409	-2.169594	-0.692294
C	-3.459414	-0.394344	1.914148
H	-3.831776	-0.780997	2.861268
C	-3.979901	0.629352	1.198336
H	-4.853506	1.225825	1.45645
C	1.924642	2.701952	1.21607
C	1.033997	3.180566	2.206221
C	0.736029	4.551191	2.239208
H	0.049997	4.928064	3.001189
C	1.305101	5.442886	1.33416
H	1.066528	6.508037	1.384798
C	2.166886	4.959695	0.352014
H	2.597653	5.654742	-0.372704
C	2.479913	3.596852	0.264887
C	3.394404	3.121725	-0.859006
H	3.548402	2.040903	-0.739271

C	2.72737	3.338921	-2.227064
H	1.778443	2.785282	-2.297392
H	3.387354	2.995421	-3.037302
H	2.508103	4.40402	-2.404217
C	4.78115	3.782663	-0.796768
H	4.719194	4.873654	-0.939747
H	5.436235	3.381203	-1.586268
H	5.271296	3.598596	0.172149
C	0.406639	2.270221	3.253486
H	0.850244	1.274099	3.124093
C	0.711888	2.737377	4.687732
H	1.793291	2.846147	4.862991
H	0.31999	2.015621	5.421501
H	0.242763	3.710056	4.904928
C	-1.11038	2.143167	3.042419
H	-1.607498	3.124427	3.100618
H	-1.563627	1.488676	3.801524
H	-1.341618	1.7181	2.056378
C	3.028385	-2.098717	-1.458466
C	2.663294	-3.451908	-1.270053
C	2.719896	-4.321861	-2.36774
H	2.44088	-5.369616	-2.235091
C	3.104339	-3.870911	-3.627001
H	3.148504	-4.564057	-4.470966
C	3.400598	-2.52143	-3.81409
H	3.663529	-2.172847	-4.813296
C	3.356495	-1.610853	-2.749262
C	3.647637	-0.131004	-2.983253
H	2.97376	0.435754	-2.319951
C	3.340332	0.324939	-4.415659
H	4.056586	-0.091289	-5.142388
H	3.408918	1.420209	-4.489184
H	2.326526	0.027475	-4.724251
C	5.087446	0.245523	-2.592974
H	5.278977	0.079287	-1.523996
H	5.280364	1.309773	-2.801407
H	5.813688	-0.349747	-3.170489
C	2.108349	-3.958616	0.053288
H	2.314909	-3.203497	0.823739
C	2.738683	-5.276634	0.528261
H	2.362312	-5.535744	1.531103
H	3.837562	-5.214542	0.581096
H	2.486177	-6.115937	-0.13955

C	0.580869	-4.088192	-0.057423
H	0.122591	-3.129422	-0.341743
H	0.145876	-4.409517	0.89737
H	0.308496	-4.830729	-0.825378
C	-3.845152	1.768935	-0.972778
C	-4.919873	1.266564	-1.749821
C	-5.506256	2.113265	-2.698923
H	-6.330826	1.743929	-3.311864
C	-5.044264	3.415995	-2.886224
H	-5.513657	4.061637	-3.633083
C	-3.977656	3.886598	-2.12616
H	-3.611543	4.903774	-2.283924
C	-3.358022	3.08029	-1.158666
C	-2.182468	3.638201	-0.371993
H	-1.845904	2.863674	0.327453
C	-2.586515	4.857588	0.471863
H	-2.921164	5.696921	-0.159647
H	-1.728347	5.207047	1.065866
H	-3.408377	4.610025	1.163025
C	-0.998862	3.950943	-1.300397
H	-0.71167	3.055826	-1.8723
H	-0.12888	4.274508	-0.713867
H	-1.24675	4.755027	-2.013128
C	-5.384947	-0.182707	-1.638603
H	-5.045339	-0.581019	-0.673082
C	-6.912396	-0.338202	-1.656351
H	-7.38875	0.289904	-0.887158
H	-7.187841	-1.386911	-1.459683
H	-7.347679	-0.066144	-2.631429
C	-4.725831	-1.028175	-2.743192
H	-5.027297	-0.669254	-3.740823
H	-5.02334	-2.085137	-2.656457
H	-3.627051	-0.976279	-2.688602
C	-1.962458	-2.293357	1.775924
C	-2.668526	-3.395108	1.231103
C	-2.466978	-4.660635	1.798266
H	-3.015434	-5.517833	1.401014
C	-1.577045	-4.846917	2.855109
H	-1.439149	-5.840916	3.288109
C	-0.843446	-3.765249	3.336244
H	-0.123642	-3.919457	4.14359
C	-1.016787	-2.477296	2.807231
C	-0.196193	-1.324461	3.360111

H	-0.470394	-0.431423	2.786439
C	-0.528101	-1.050208	4.834942
H	-1.600446	-0.838483	4.970091
H	0.041297	-0.184306	5.206095
H	-0.274478	-1.913311	5.471712
C	1.308515	-1.553813	3.156067
H	1.662513	-2.454237	3.682636
H	1.891775	-0.698922	3.528259
H	1.550424	-1.676401	2.090306
C	-3.627494	-3.251121	0.055303
H	-3.562653	-2.216948	-0.309215
C	-3.215318	-4.156936	-1.116119
H	-2.182934	-3.943162	-1.431557
H	-3.876728	-3.991847	-1.980824
H	-3.278106	-5.224376	-0.849999
C	-5.08732	-3.48239	0.476176
H	-5.243283	-4.512054	0.838152
H	-5.765687	-3.318692	-0.376925
H	-5.380455	-2.789815	1.280101

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