The heterocubane $[TerSnAs]_4$

Supporting Information

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Contents

1. Syntheses

General methods. All reactions and product manipulations were carried out under an inert atmosphere of argon or dinitrogen using standard Schlenk-line or glovebox techniques (MBraun UNIlab glovebox maintained at < 0.1 ppm H_2O and < 0.1 ppm O_2). The irradiation experiments were conducted with a medium pressure mercury lamp and an immersion well reactor obtained from Photochemical Reactors Ltd.

NMR spectra were acquired at 298 K at 400.2 (^{1}H), 100.6 (^{13}C), 162.0 (^{31}P) and 149.3 (^{119}Sn) MHz, respectively, on a Bruker Avance 400 HD Ascend NMR spectrometer. ^{1}H and ^{13}C NMR spectra were referenced to the most downfield solvent resonance.[1] Elemental analyses were carried out by Elemental Microanalyses Ltd. (Devon, U.K.). Samples (approx. 10 mg) were submitted in sealed Pyrex ampoules.

Hexane (hex; Sigma-Aldrich, HPLC grade) and toluene (tol; Sigma-Aldrich, HPLC grade) were purified using an MBraun SPS-800 solvent system. Tetrahydrofuran (THF; Sigma-Aldrich, HPLC grade) was distilled over sodium metal/benzophenone. All dry solvents were stored under argon in gas-tight ampoules over activated 3 Å molecular sieves. [D_8]-Toluene (Sigma-Aldrich, 99.5%), [D_8]-THF (Sigma-Aldrich, 99.5%) and C_6D_6 (Sigma-Aldrich, 99.5%) were dried over CaH_2 and vacuum distilled before use. Other starting materials were prepared according to published procedures: TerSnCl,[2] [Na(dioxane)$_x$]PCO (x = 2.8),[3] [Na(dioxane)$_x$]AsCO (x = 3.3),[4] [Na(18-crown-6)]AsCO.[5]

1.1. [TerSnAs]$_4$ (**4As**)

To a mixture of TerSnCl (95 mg, 0.203 mmol) and [Na(dioxane)$_{3.3}$]AsCO (89 mg, 0.213 mmol), 3 ml of cold toluene (–30 °C) were added. The mixture was stirred for one hour and then warmed to room temperature. The resulting dark red suspension was filtered, all volatiles were removed *in vacuo* and the crude product was obtained. Recrystallisation from toluene afforded **4As** as an orange crystalline product (42 mg, 0.021 mmol, 41%).

^{1}H NMR (C_6D_6, 400 MHz): 2.12 (s, 12 H; *o*-CH_3), 2.17 (s, 12 H; *p*-CH_3), 6.66 (d, $^3J_{H–H}$ = 7.6 Hz, 2 H; *m*-C*H*), 6.85 (s, 4 H; *m*-CH_{Mes}), 7.05 (t, $^3J_{H–H}$ = 7.6 Hz, 1 H; *p*-C*H*). **^{13}C NMR** (C_6D_6, 100 MHz): 23.09 (s; *p*-CH_3), 25.82 (s; *o*-CH_3), 129.37 (s; *p*-C*H*, *m*-CH_{Mes}), 129.93 (s; *m*-CH_{Mes}), 136.14 (s), 136.56 (s), 139.55 (s), 149.73 (s). **^{119}Sn NMR** (C_6D_6): −693 (s, ^2J(^{119}Sn–^{117}Sn) = 1114 Hz). Satisfactory elemental analyses could not be obtained.

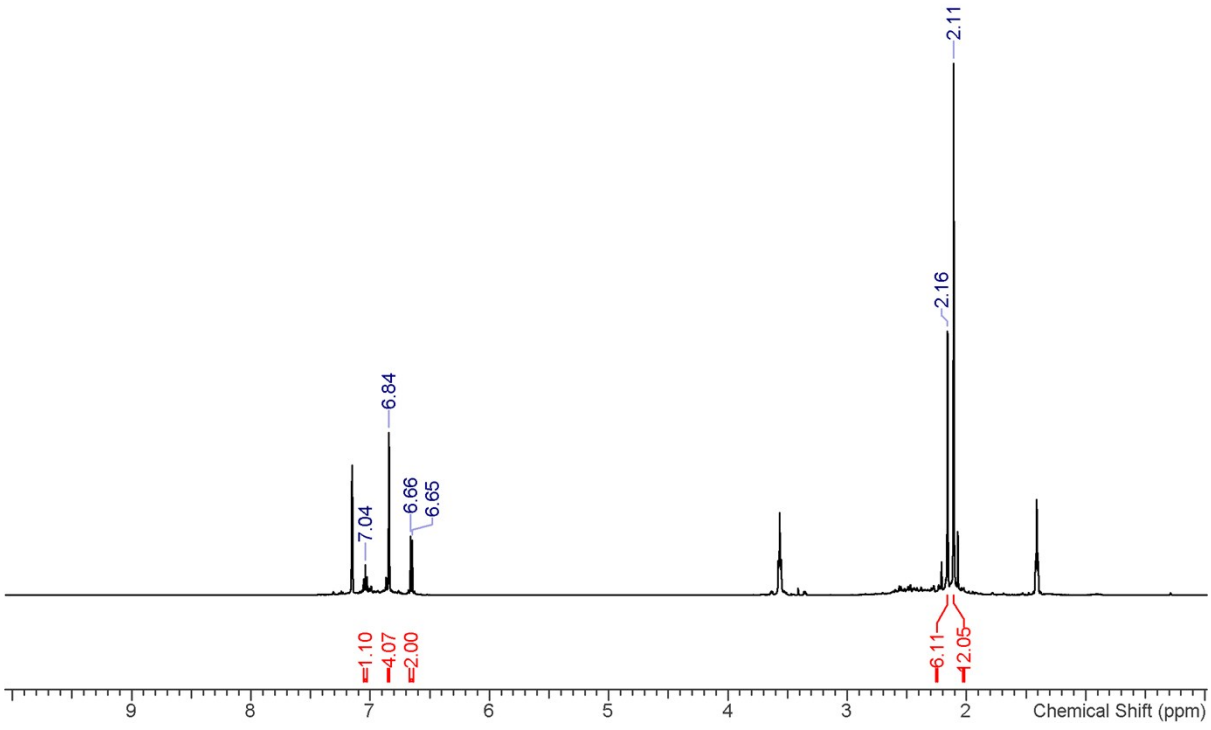


Figure S1. ^{1}H NMR spectrum of **4As**.

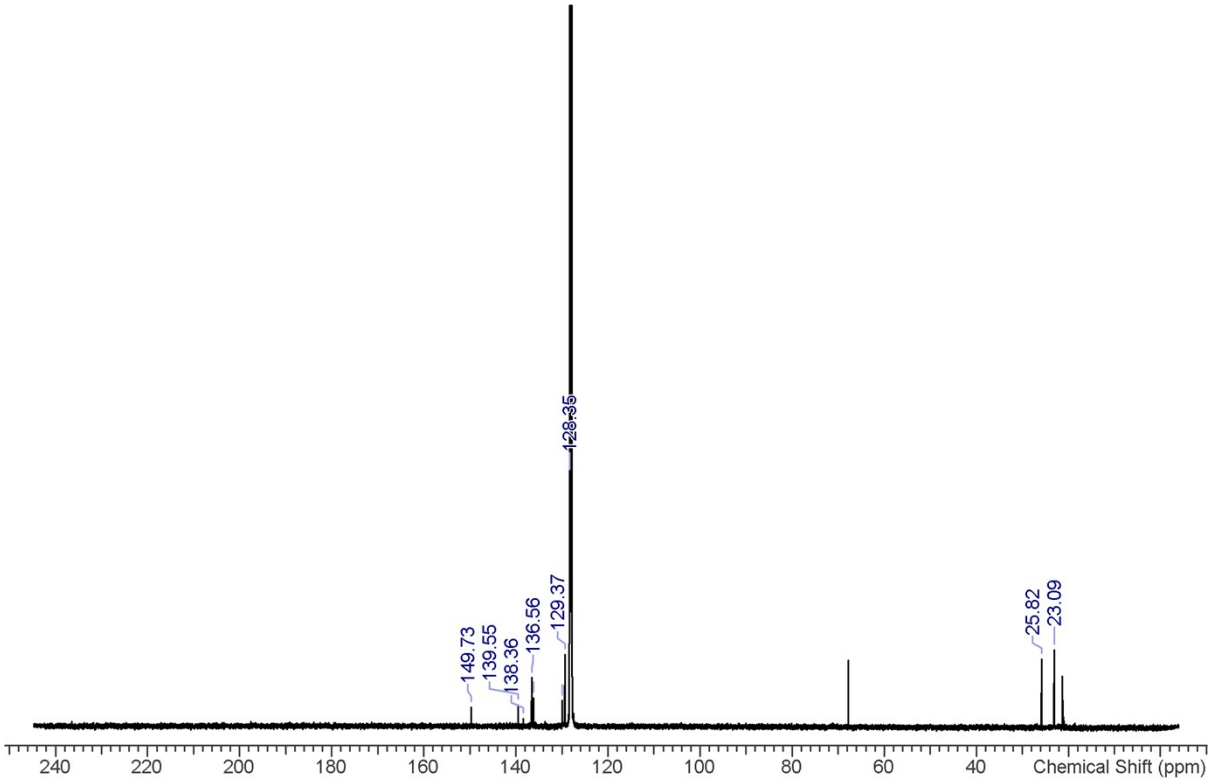


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **4As**.

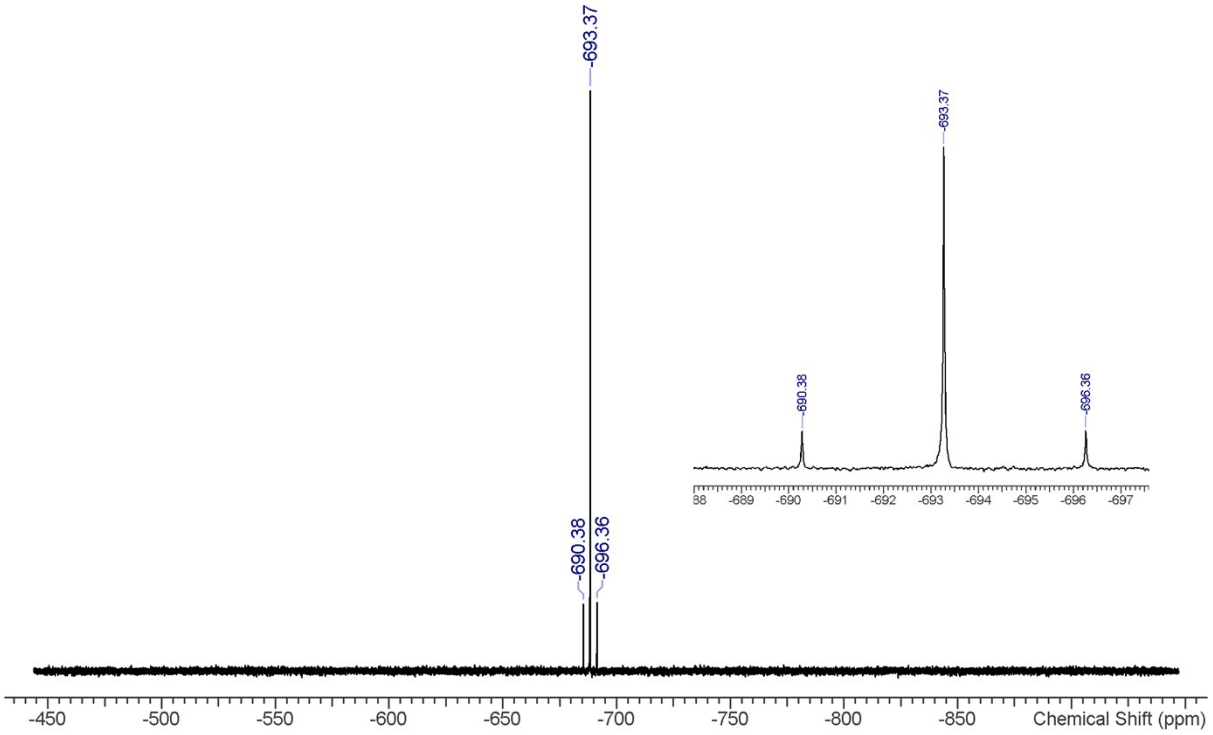


Figure S3. ^{119}Sn NMR spectrum of **4As** showing the ^{117}Sn satellites on the ^{119}Sn NMR resonance.

1.2. Attempted synthesis of $[TerSnP]_4$ (**4P**)

To a solid mixture of TerSnCl (450 mg, 0.96 mmol) and $[Na(dioxane)_{2.8}]PCO$ (315 mg, 0.96 mmol), 10 ml of toluene were added. The mixture was stirred for one hour and turned dark yellow in the process. The suspension was filtered, all volatiles were removed *in vacuo* and the crude product (TerSnPCO) was obtained. The product can be characterised by NMR spectroscopy but is not stable for prolonged periods of time in solution. After standing overnight in solution at room temperature, TerSnPCO had completely decomposed and the solution had turned dark red (^{31}P NMR spectrum is depicted below). Various attempts of crystallisation were undertaken from common solvents such as Et_2O, hexane, benzene, toluene, THF. Whilst various by-products and decomposition products could be crystallised (see below, section 1.2.1 and 1.2.2), their formation is difficult to control.

Following the same protocol, [Na(18-crown-6)]PCO can be used in equimolar amounts to TerSnCl. In polar solvents such as THF or pyridine, the intermediate TerSnPCO is considerably less stable and decomposes completely within an hour.

1.2.1. TerSnPCO (**2P**)

^{1}H NMR (C_6D_6, 400 MHz): 2.28 (s, 6 H; *p*-CH_3), 2.46 (s, 18 H; *o*-CH_3), 6.93 (s, 4 H; *m*-CH_{Mes}), 7.11 (d, $^{3}J_{H–H}$ = 7.5 Hz, 2 H; *m*-CH_3), 7.32 (t, $^{3}J_{H–H}$ = 7.5 Hz, 1 H; *p*-C*H*). **^{31}P**{^{1}H} **NMR** (C_6D_6, 126 MHz): –347 (br s), –332 (br s). **^{119}Sn NMR** (C_6D_6, 149 MHz): +213 (br s), +283 (br s).

The occurrence of two resonances in both ^{31}P and ^{119}Sn NMR spectra can be due to dimeric nature of [TerSnPCO] in solution and the interconversion of cis and trans isomer or the interconversion of oligomers.

From a reaction mixture with THF/toluene sharp resonances were observed in the ^{31}P and ^{119}Sn NMR spectra but also reduced the lifetime of the species.

^{31}P{^{1}H} **NMR** (C_6D_6 capillary, 126 MHz): –346 (s, J_{PSn} = 835 Hz). **^{119}Sn NMR** (C_6D_6, 149 MHz): +33 (t, J_{PSn} = 835 Hz).

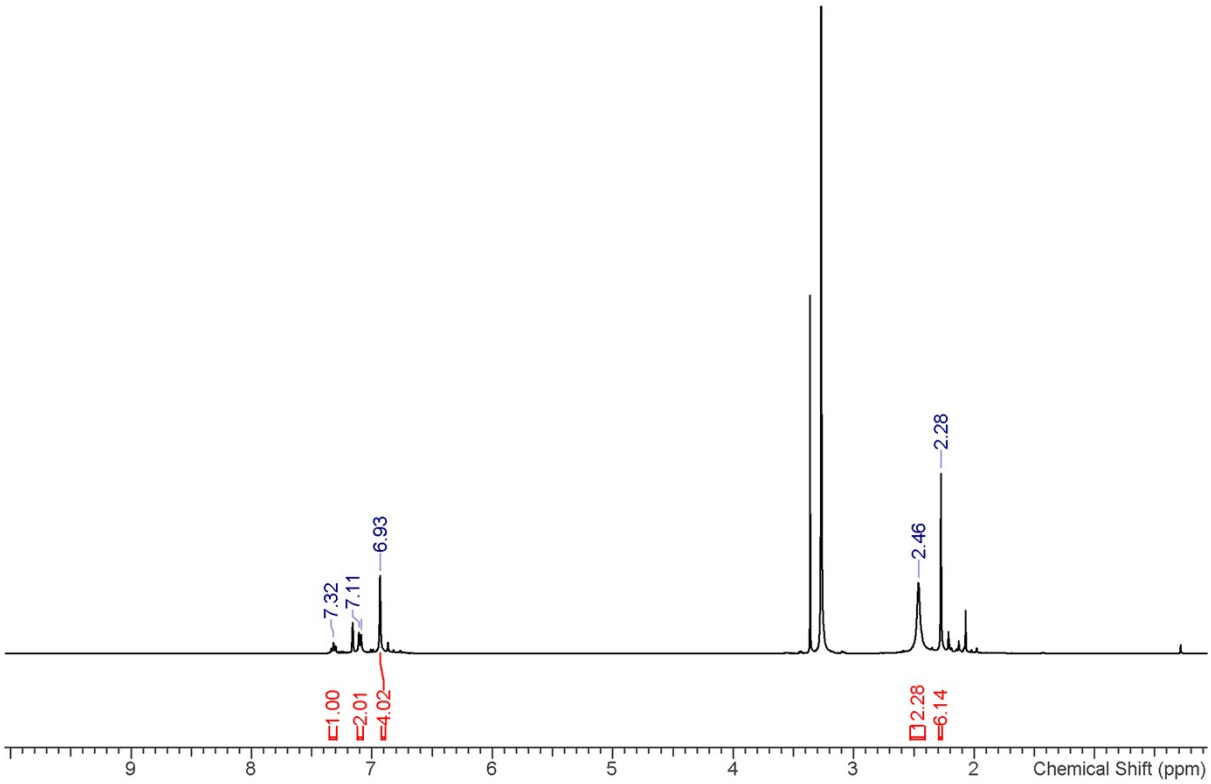
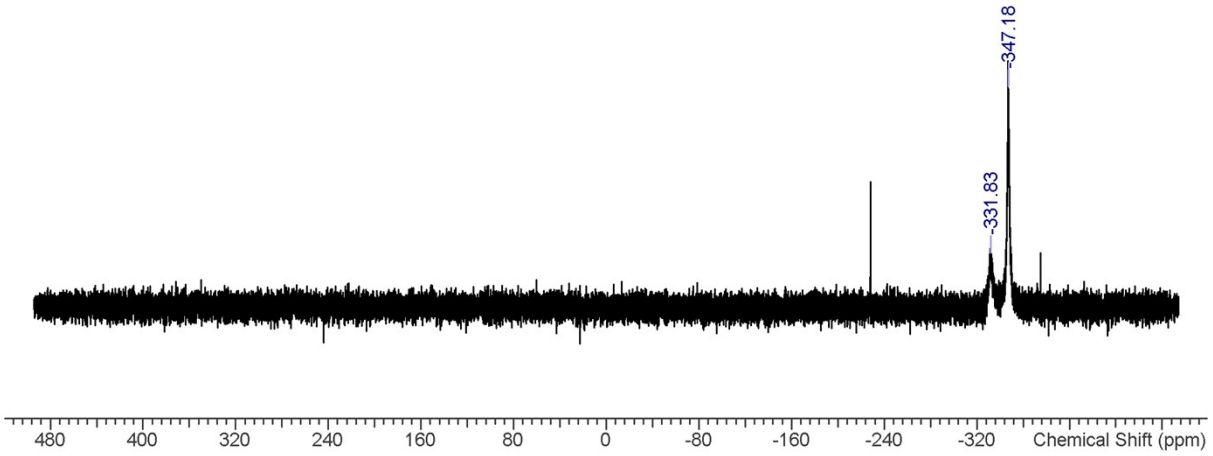


Figure S4. ^{1}H NMR spectrum of **2P**.



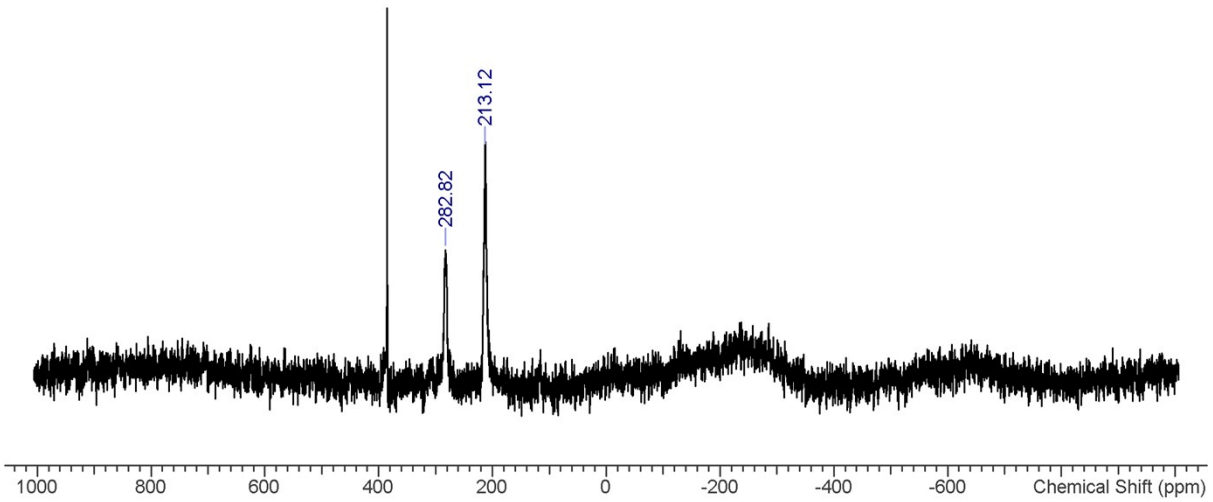
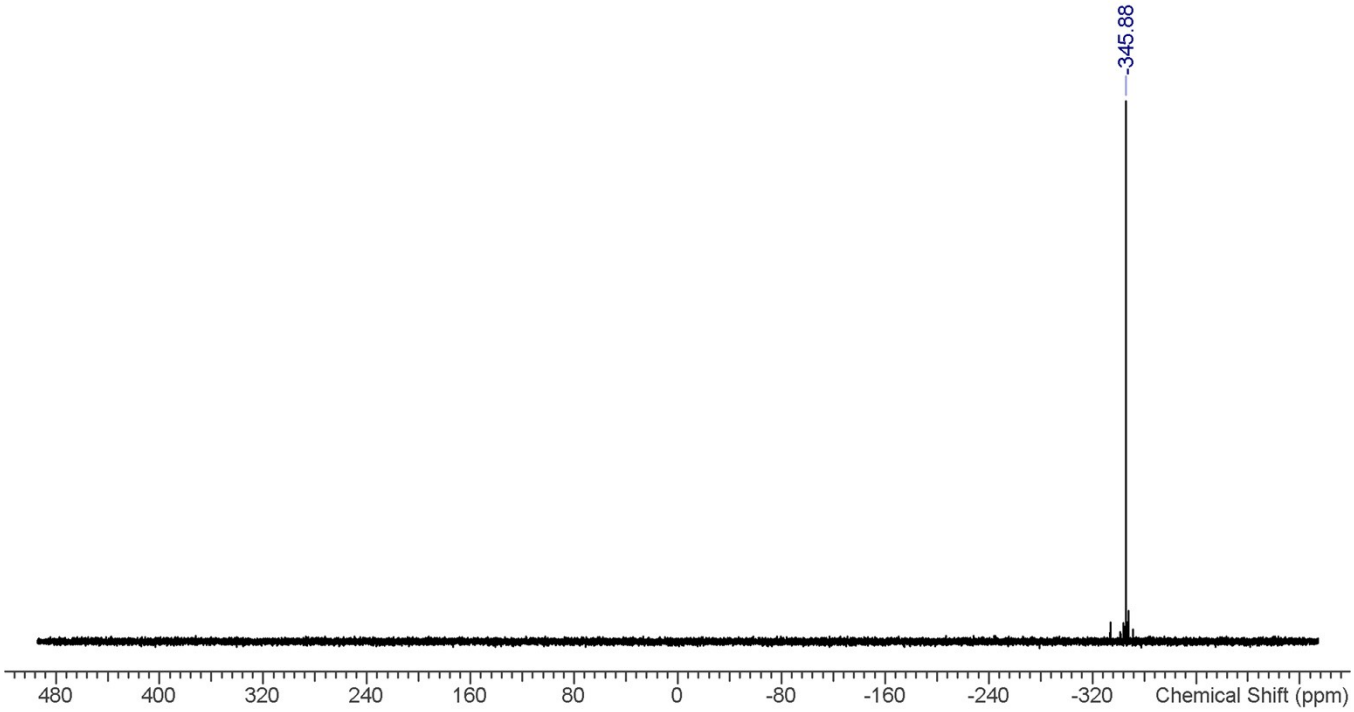


Figure S5. $^{31}P\{^{1}H\}$ and ^{119}Sn NMR spectrum of **2P** in C_6D_6.



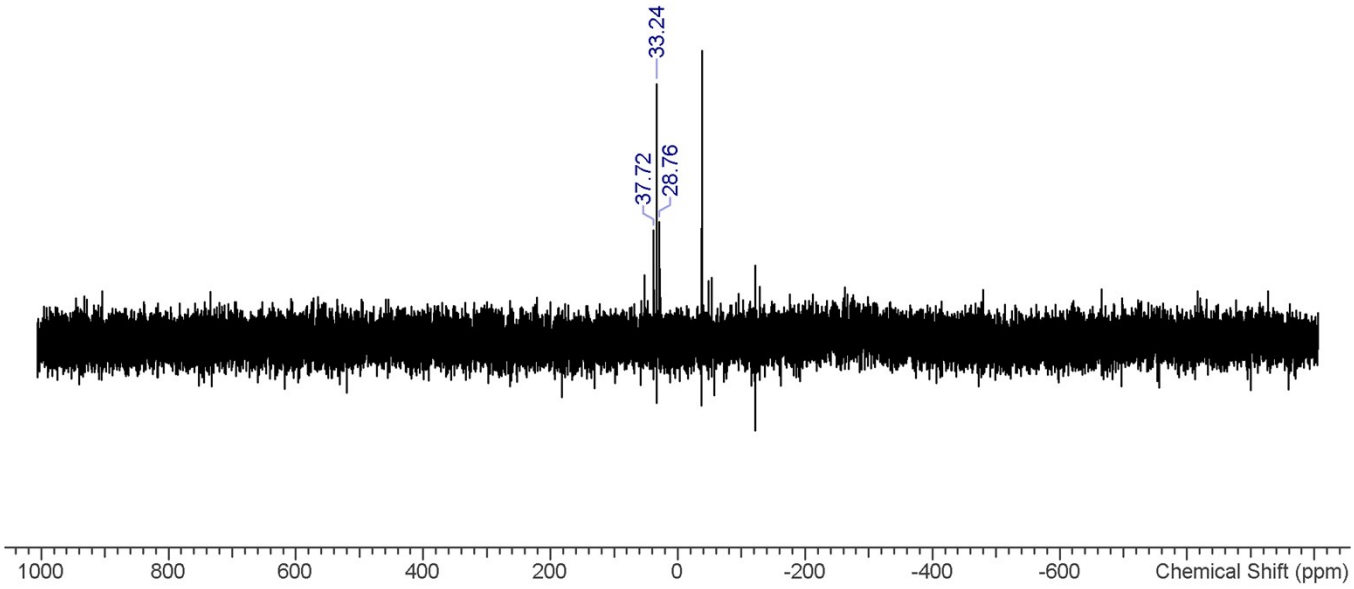


Figure S6. $^{31}P\{^{1}H\}$ and ^{119}Sn NMR spectrum of **2P** in C_6D_6 with 10% THF.

1.2.2. Compound **5**

^{31}P{^{1}H} **NMR** (C_6D_6, 126 MHz): –81, +114, +204, +286. **^{119}Sn NMR** (C_6D_6, 149 MHz): –376, –10, +119, +501.

^{31}P{^{1}H} **NMR** ([D_8]-toluene, 126 MHz, 193 K): Two sets (T_C = 200 K): +290/+268, +208/+189, +115/+100, –63/–91.

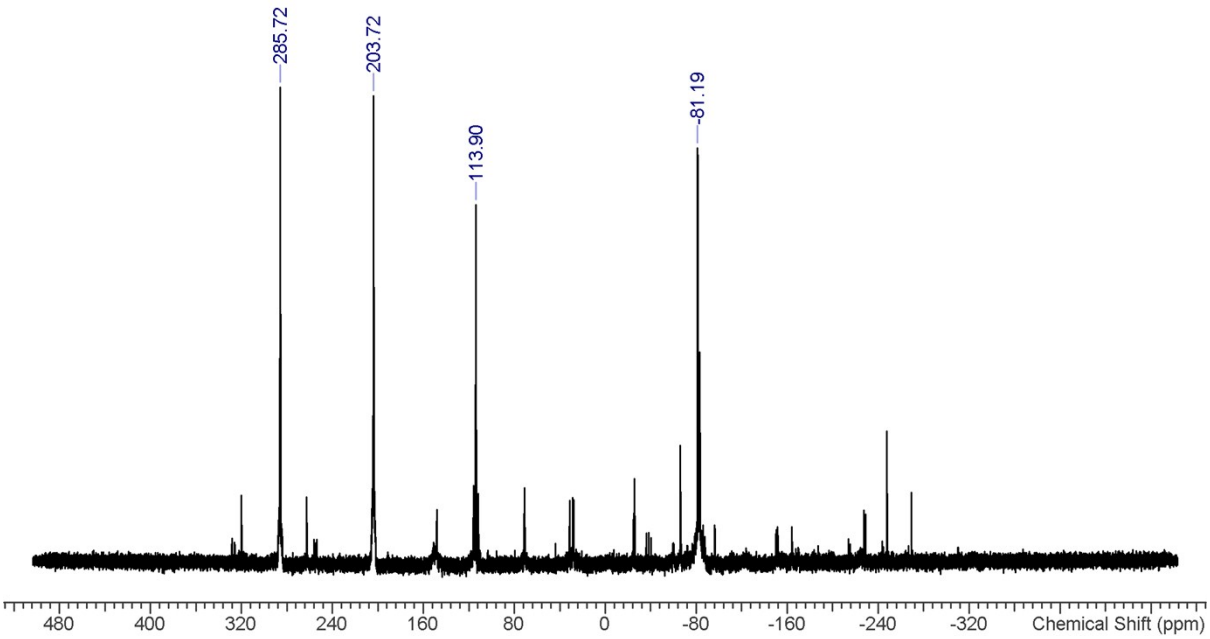


Figure S7. ^{31}P{^{1}H} NMR spectrum of crude **5**.

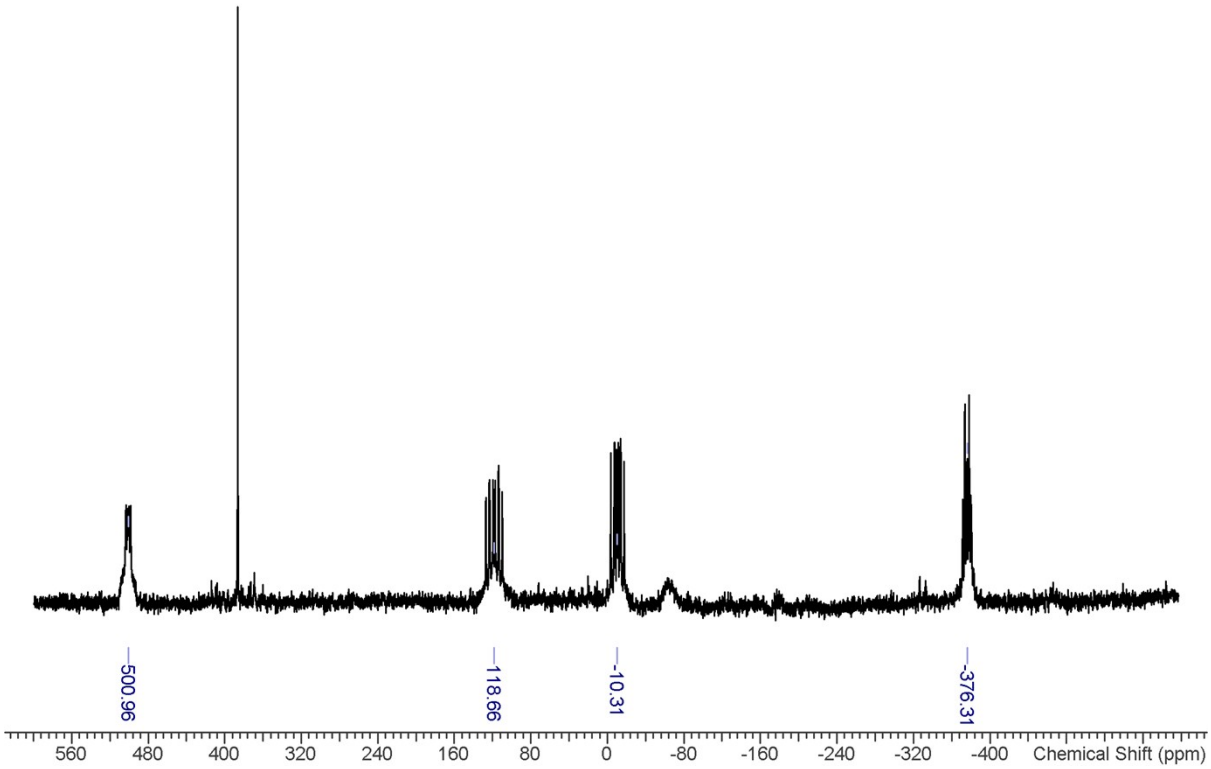


Figure S8. ^{119}Sn NMR spectrum of crude **5**.

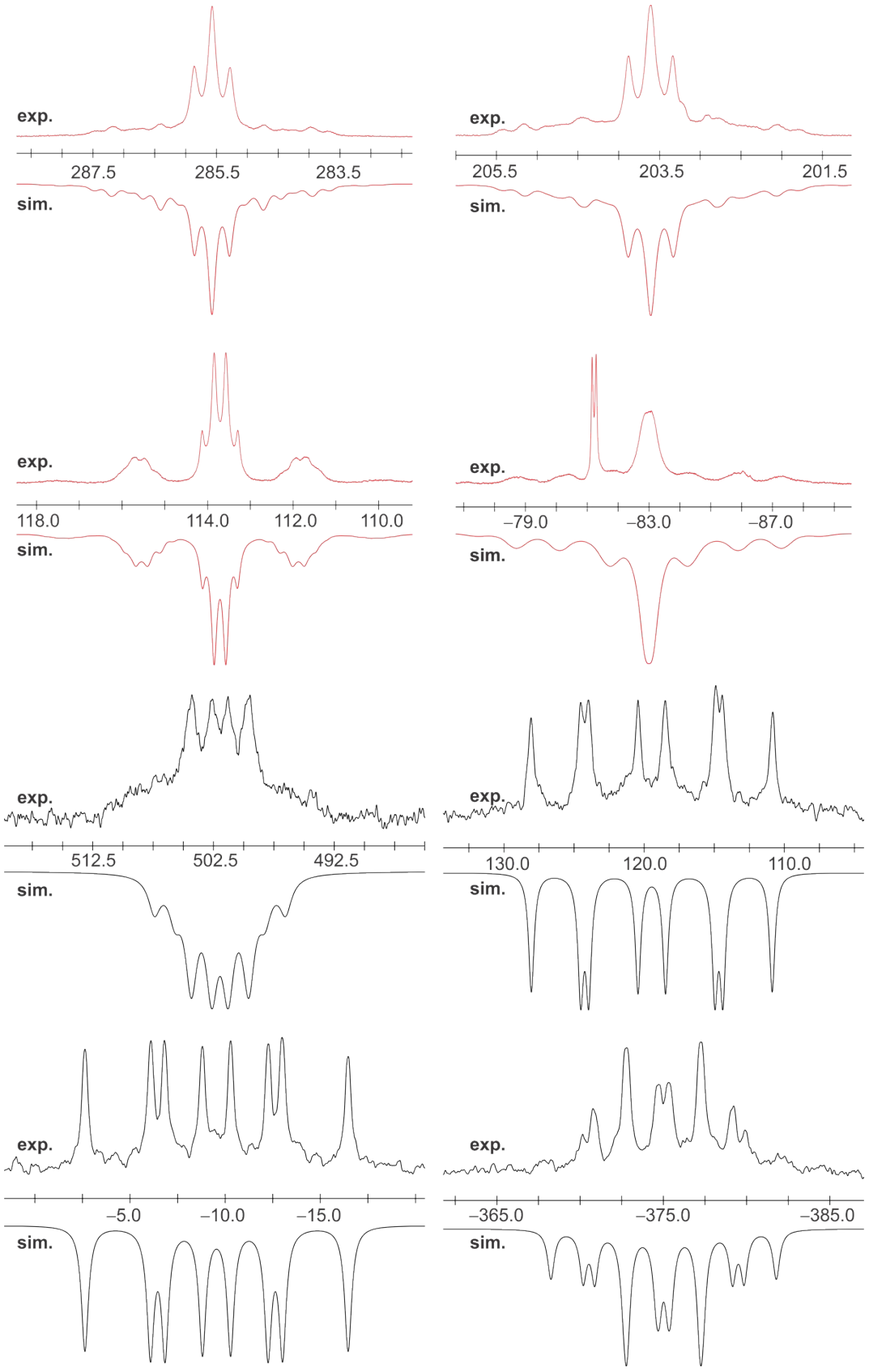


Figure S9. Sections of the simulated $^{31}P\{^{1}H\}$ (red, top) and ^{119}Sn NMR (green, bottom) spectra of crude **5**.

1.2.3. Compound **6**

^{31}P{^{1}H} **NMR** ([D_8]-toluene, 126 MHz, 278 K): –226, –161, +293.

^{31}P{^{1}H} **NMR** ([D_8]-toluene, 126 MHz, 193 K): –263, –202, – 162, +282.

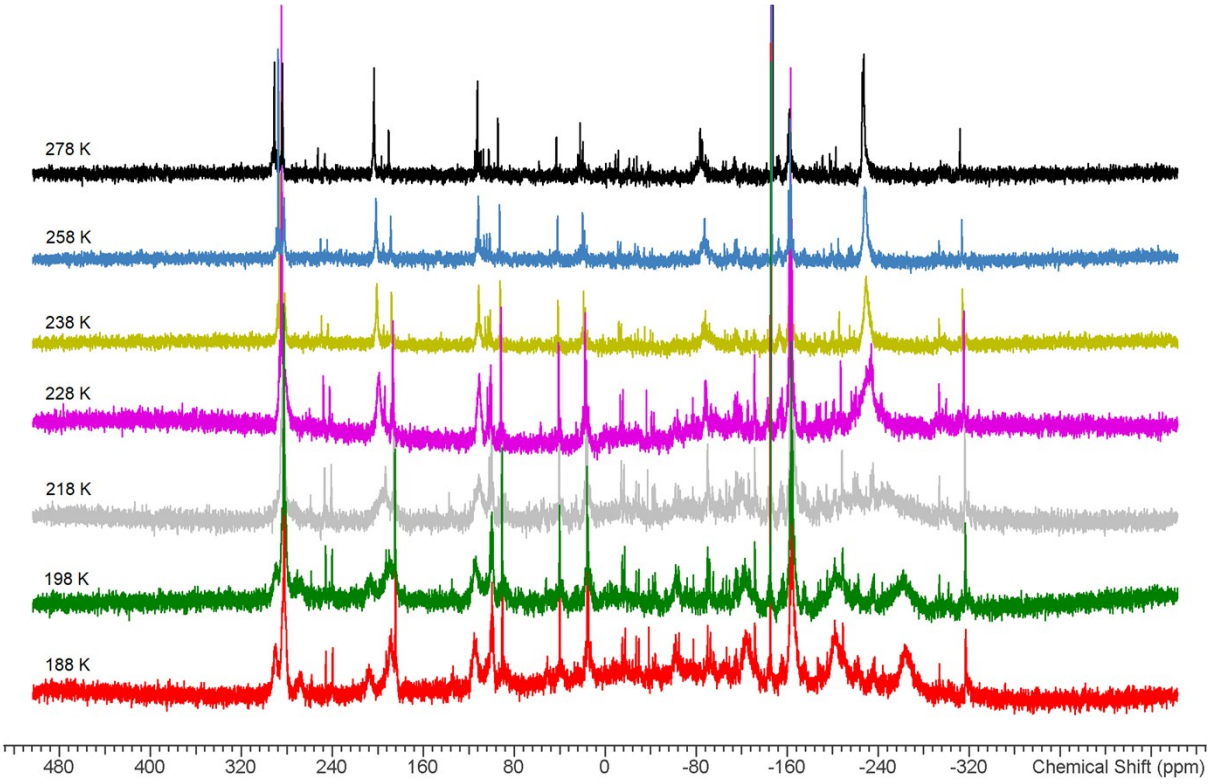


Figure S10. VT ^{31}P{^{1}H} NMR spectra of redissolved crystals of **6**.

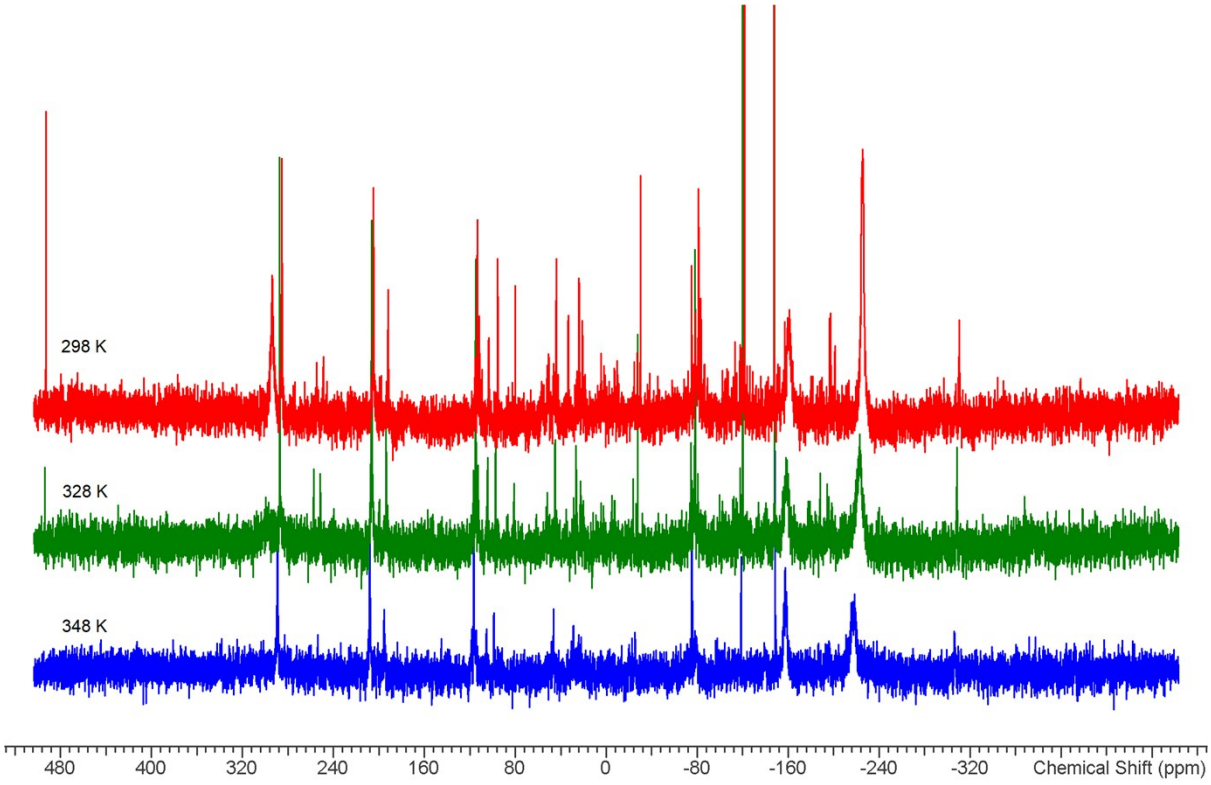


Figure S11. VT $^{31}P\{^{1}H\}$ NMR spectra of redissolved crystals of **6** (heated to 348 K initially and then cooled). Notably, decomposition sets in and Ter_2P_2 is formed (+492 ppm).

1.2.4. [Na(18-crown-6)][$Ter_4Sn_4P_5$] (**7**)

^{1}H NMR ([D_8]-THF, 400 MHz): 1.68 (s, 6 H; CH_3), 1.93 (s, 18 H; CH_3), 2.16 (s, 12 H; CH_3), 3.54 (s; 18-crown-6 CH_2), 6.60 (d, $^3J_{H–H}$ = 7.3 Hz, 4 H; *o*-C*H*), 6.66 (d, $^3J_{H–H}$ = 7.5 Hz, 4 H; *o*-C*H*), 6.70 (s, 4 H; CH_{Mes}), 7.01 (t, $^3J_{H–H}$ = 7.3 Hz, 2 H; *p*-C*H*), 7.09 (t, $^3J_{H–H}$ = 7.5 Hz, 2 H; *p*-C*H*). **^{31}P**{^{1}H} **NMR** ([D_8]-THF, 126 MHz): –115.8, –58.6, +2.4. **^{119}Sn NMR** ([D_8]-THF, 149 MHz): –179.5 (br t), +1.6 (br d, $^1J_{Sn–P}$ = 1300 Hz).

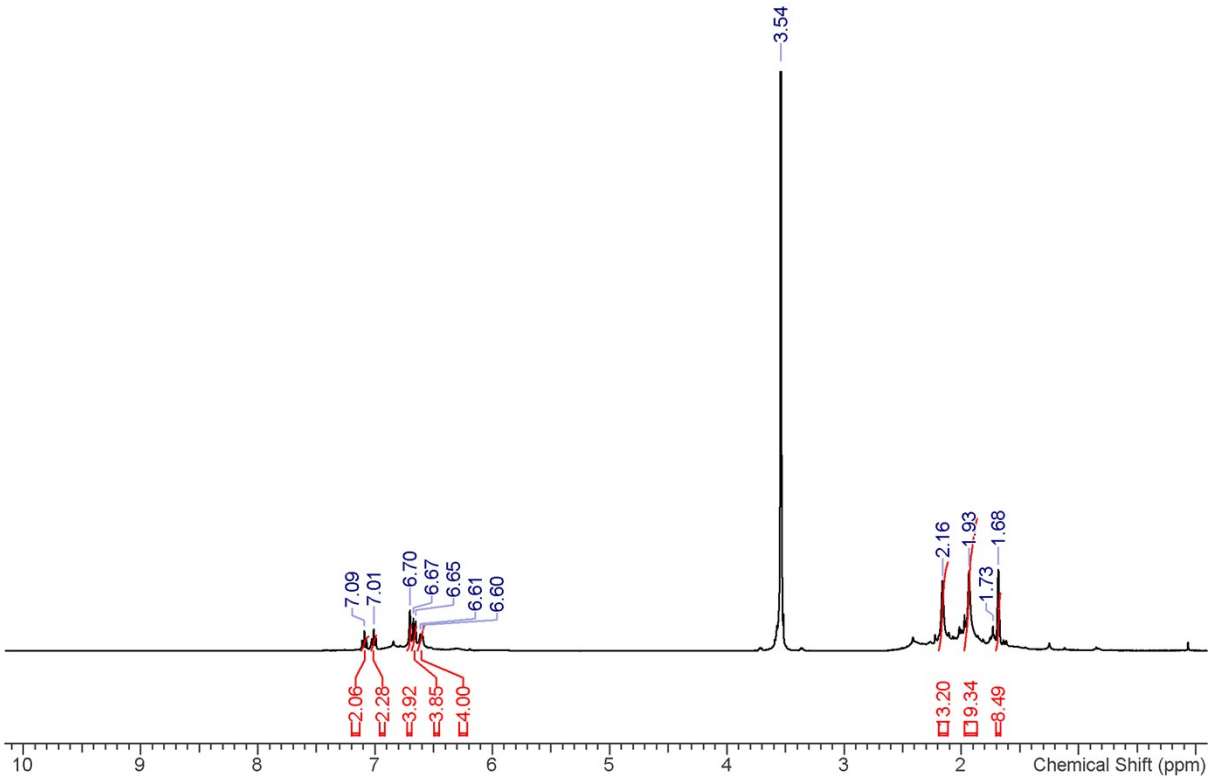


Figure S12. ^{1}H NMR spectrum of **7**.

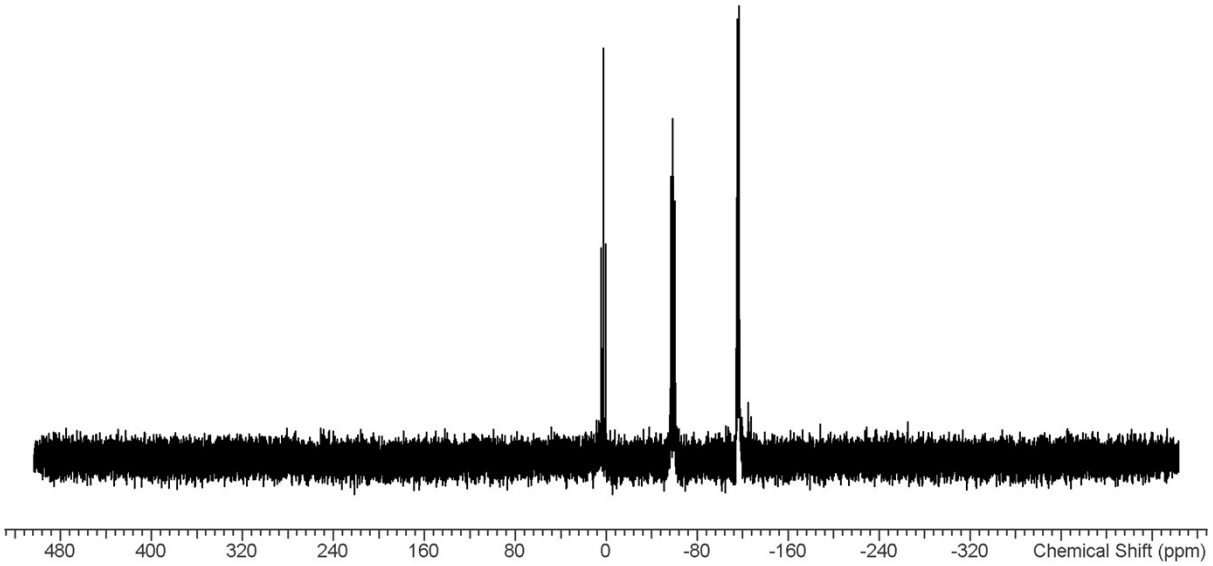


Figure S13. $^{31}P\{^{1}H\}$ NMR spectrum of **7**.

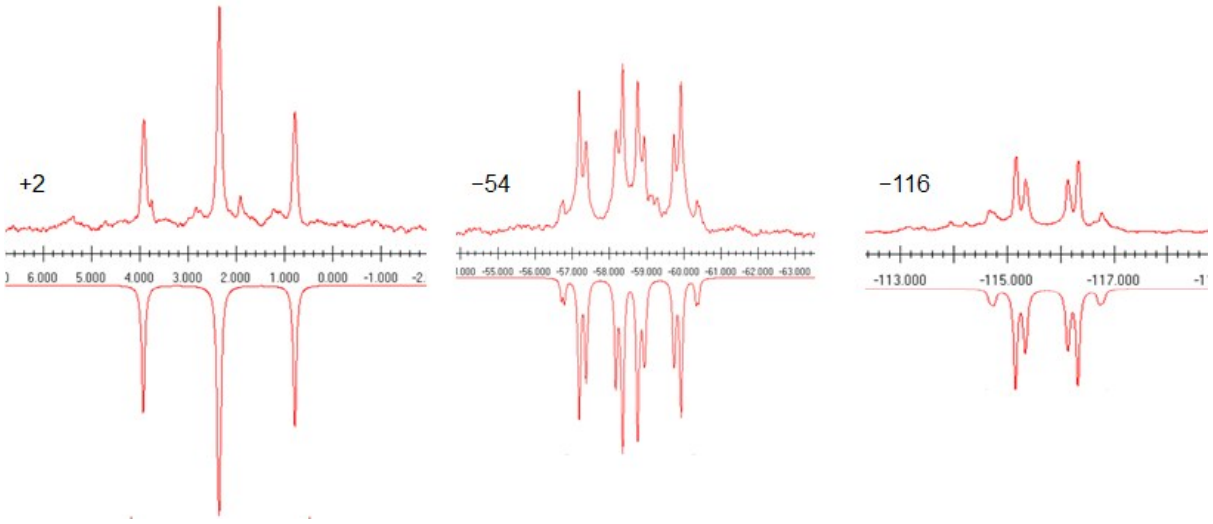


Figure S14. $^{31}P\{^{1}H\}$ NMR spectrum of **7** and simulated pattern.

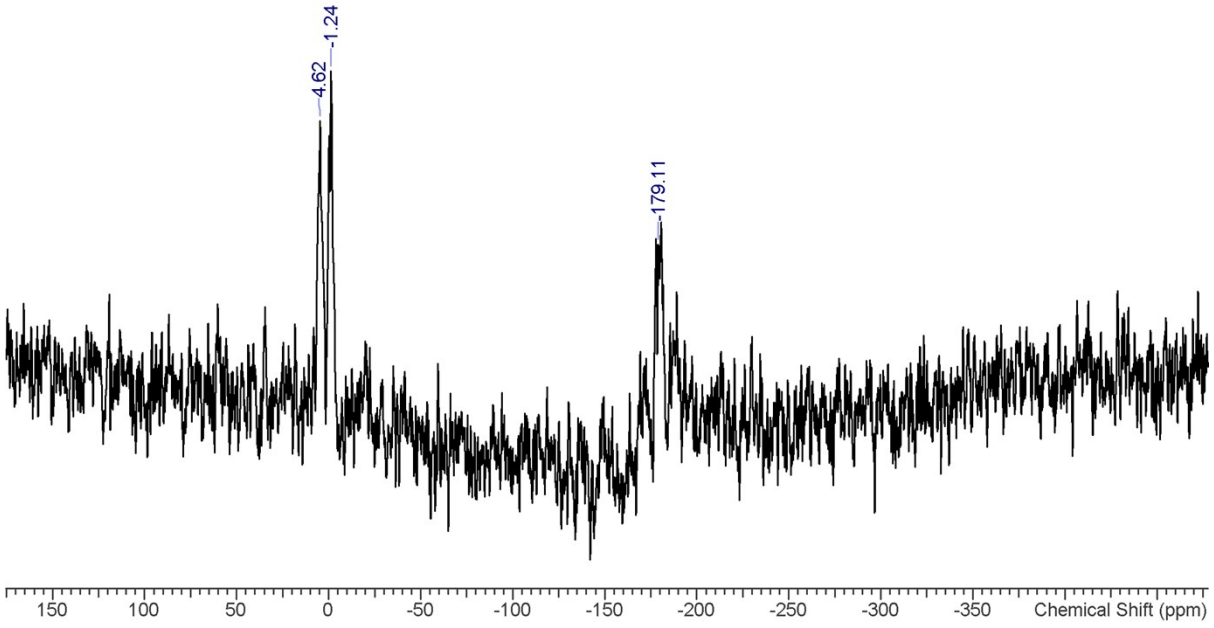


Figure S15. ^{119}Sn NMR spectrum of **7**.

2. Crystallography

Single crystal X-ray structure determination: Single-crystal X-ray diffraction data were collected using an Oxford Diffraction Supernova dual-source diffractometer equipped with a 135 mm Atlas CCD area detector. Crystals were selected under Paratone-N oil, mounted on micromount loops and quench-cooled using an Oxford Cryosystems open flow N_2 cooling device.[6] Data were collected at 150 K using mirror monochromated Cu K_α radiation (λ = 1.5418 Å; Oxford Diffraction Supernova). Data collected on the Oxford Diffraction Supernova diffractometer were processed using the CrysAlisPro package, including unit cell parameter refinement and inter-frame scaling (which was carried out using SCALE3 ABSPACK within CrysAlisPro).[7] Equivalent reflections were merged and diffraction patterns processed with the CrysAlisPro suite. Structures were subsequently solved using direct methods and refined on F^2 using the ShelXL 2013 package and ShelXle.[8,9]

Table S1. Selected X-ray data collection and refinement parameters for **4As**·1.5tol, **4As**·1.23hex, **6**·OEt_2, [Na(18-c-6)$_2$(THF)][**7**]·3C_6H_6 and **8**·1.5tol.

	4As·1.5tol	**4As**·1.23hex	**6**·OEt_2	[Na(18-c-6)$_2$(THF)][**7**]·3C_6H_6	**8**·1.5tol
Formula	$C_{106.5}H_{112}As_4Sn_4$	$C_{103.37}H_{117.2}As_4Sn_4$	$C_{100}H_{110}OP_4Sn_4$	$C_{142}H_{174}NaO_{13}P_5Sn_4$	$C_{107.5}H_{112}NaOP_5Sn_4$
CCDC	1840063	1840064	1840065	1840066	1840067
Fw [g mol^{-1}]	2166.39	2134.04	1926.51	2741.40	2072.56
Crystal system	triclinic	triclinic	monoclinic	monoclinic	triclinic
Space group	*P*–1	*P*–1	$P2_1/n$	$P2_1/c$	*P*–1
a (Å)	14.1569(3)	14.1237(4)	13.6543(2)	26.2345(4)	14.5008(4)
b (Å)	14.5547(3)	14.5696(3)	15.3818(3)	18.0987(2)	15.6338(4)
c (Å)	24.0923(5)	24.1788(4)	42.7159(9)	29.6611(4)	23.2169(6)
α (°)	81.922(2)	81.378(2)	90	90	89.608(2)
β (°)	85.928(2)	86.140(2)	95.234(2)	106.370(2)	87.993(2)
γ (°)	71.265(2)	71.879(2)	90	90	63.640(3)
V (Å^3)	4652.75(18)	4674.09(19)	8934.1(3)	13512.5(3)	4712.9(2)
Z	2	2	4	4	2
Radiation, λ (Å)	Cu Kα, 1.54184	Cu Kα, 1.54184	Cu Kα, 1.54184	Cu Kα, 1.54184	Cu Kα, 1.54184
Temp (K)	150(2)	150(2)	150(2)	150(2)	150(2)
ρ_{calc} (g cm^{-3})	1.546	1.516	1.432	1.348	1.460
μ (mm^{-1})	10.368	10.309	9.818	6.861	9.547
Reflections collected	53723	54480	55508	79084	50400
Independent reflections	19219	19325	18413	27955	19413
Parameters	1193	1143	1270	1776	1054
R(int)	0.0344	0.0281	0.0583	0.0428	0.0395
R1/wR2,[a] $I \geq 2\sigma I$ (%)	3.36/8.43	3.05/7.54	7.34/16.89	5.50/14.59	6.47/16.42
R1/wR2,[a] all data (%)	3.81/8.70	3.18/7.61	9.22/17.65	7.52/16.18	7.50/17.43
GOF	1.079	1.141	1.107	1.066	1.031

[a] $R1 = [\Sigma||F_o| - |F_c||]/\Sigma|F_o|$; $wR2 = \{[\Sigma w[(F_o)^2 - (F_c)^2]^2]/[\Sigma w(F_o^2)^2\}^{1/2}$; $w = [\sigma^2(F_o)^2 + (AP)^2 + BP]^{-1}$, where $P = [(F_o)^2 + 2(F_c)^2]/3$ and the A and B values are 0.0393 and 8.68 for **4As**·1.5tol, 0.0293 and 7.96 for **4As**·1.23hex, 0.0370 and 65.13 for **6**·OEt_2, 0.0808 and 21.19 for [Na(18-c-6)$_2$(THF)][**7**]·3C_6H_6, and 0.0846 and 39.64 for **8**·1.5tol.

3. Computations

3.1. General considerations

Computational details. Computations were performed using Gaussian09, revision D.01, using the implemented PBE1PBE level of theory.[10] For all atoms Def2SVP basis sets were utilised. The geometry optimisation was carried out until no significant change in energy occurred. The electronic situation was analysed with NBO program.[11]

	E [a.u.]
[TerSnAs]	–3377.57070417
[TerSnAs]$_2$	–6755.28603447
[TerSnAs]$_4$	–13510.7468168
[TerSnP]	–1483.33493197
[TerSnP]$_2$	–2966.81695503
[TerSnP]$_4$	–5933.81363766

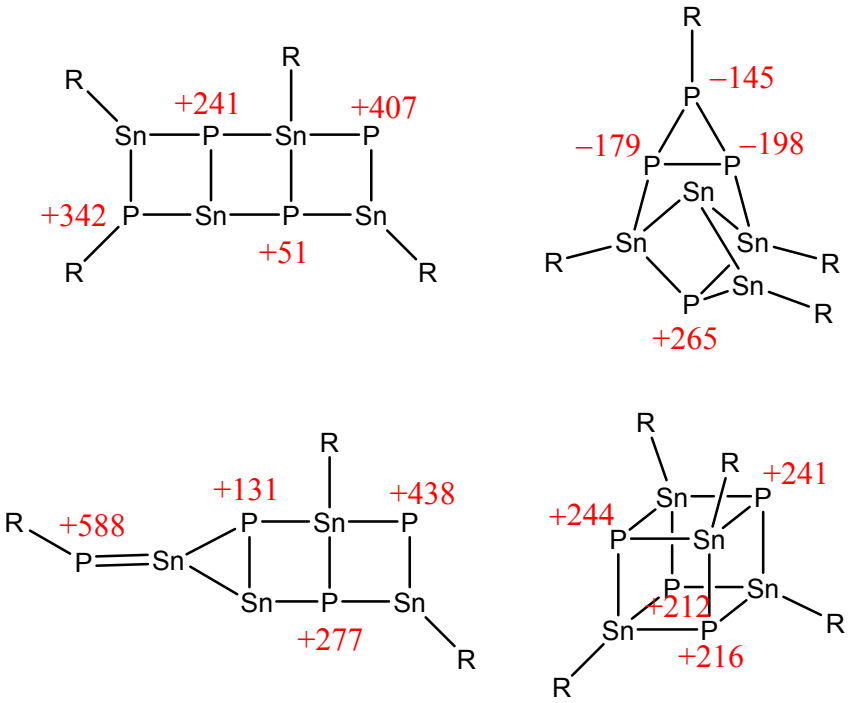


Figure S16. Selected isomers of [Ter$_4$Sn$_4$P$_4$] and their computed ^{31}P NMR resonances.

3.2. ^{119}Sn NMR

Computational details. All calculations were performed using the Amsterdam Density Functional package (ADF2016.01).[12] An augmented all-electron TZ2P Slater-type basis set of triple-ζ zeta quality was used to describe all atoms (ATZ2P). The computations were performed on the basis of Gaussian09-optimised structures using the dispersion-corrected hybrid functional revPBE-D3(BJ) at "good" numerical quality of integration. Relativistic effects were incorporated using the two-component Spin-Orbit Zeroth Order Relativistic Approximation (ZORA).[13]

3.3. Optimised Stuctures

3.3.1. TerSnAs

0 1

Sn	-0.00000300	0.87779600	-0.00004200
As	0.00000500	3.16464400	-0.00009000
C	-0.00001100	-1.26151100	-0.00007200
C	-1.22681600	-1.94303300	-0.00008500
C	-1.21102400	-3.34135600	-0.00013400
C	0.00000800	-4.03242200	-0.00015900
C	1.21103500	-3.34134000	-0.00012300
C	1.22680800	-1.94302200	-0.00007900
C	-2.48840600	-1.15283700	-0.00001800
C	-3.06231200	-0.75358200	-1.22285400
C	-4.19625000	0.05975900	-1.19838900
C	-4.77297400	0.48563600	0.00015100
C	-4.19614000	0.05967200	1.19860700
C	-3.06219800	-0.75367200	1.22290100
C	-2.45574400	-1.18109300	-2.52870900
C	-5.95883600	1.40500600	0.00024800
C	-2.45551900	-1.18130100	2.52866700
C	2.48838400	-1.15280500	-0.00001500
C	3.06215800	-0.75361200	1.22290900
C	4.19610100	0.05972200	1.19861100
C	4.77296700	0.48564600	0.00015100
C	4.19625900	0.05974900	-1.19838500
C	3.06230900	-0.75358300	-1.22284700
C	2.45551400	-1.18130700	2.52867000

C	5.95885100	1.40498700	0.00026200
C	2.45578400	-1.18115600	-2.52870300
H	-2.15878300	-3.88573800	-0.00014600
H	0.00001500	-5.12506200	-0.00019700
H	2.15879900	-3.88571400	-0.00012700
H	-4.63852800	0.37642600	-2.14742200
H	-4.63831800	0.37625600	2.14771300
H	-1.43132300	-0.79059500	-2.64337400
H	-3.05013300	-0.81963800	-3.37852900
H	-2.37940800	-2.27687800	-2.59891200
H	-6.58532300	1.25685600	-0.89109700
H	-5.63139800	2.45802000	0.00030700
H	-6.58526300	1.25675000	0.89161700
H	-2.37932600	-2.27710000	2.59882700
H	-3.04975000	-0.81978900	3.37857200
H	-1.43102600	-0.79095900	2.64321000
H	4.63825800	0.37635300	2.14771200
H	4.63853300	0.37640000	-2.14742400
H	2.38044700	-2.27716500	2.59924400
H	1.43058100	-0.79201100	2.64275400
H	3.04913700	-0.81886500	3.37860400
H	6.58536900	1.25655600	0.89153700
H	5.63144800	2.45801700	0.00053200
H	6.58523600	1.25696100	-0.89117200
H	2.38005900	-2.27697500	-2.59911600
H	3.04985700	-0.81921000	-3.37853400
H	1.43112500	-0.79122700	-2.64313800

3.3.2. $[TerSnAs]_2$

0 1

Sn	-1.48973100	-0.00014700	0.00010600
Sn	1.48966500	0.00043400	0.00003300
As	-0.00010300	0.00011800	-2.06486200
As	0.00004900	0.00014800	2.06500800
C	-3.63722700	-0.00074500	0.00022700
C	-4.31302500	1.13271600	-0.46412200
C	-5.71141300	1.12360100	-0.45933000
C	-6.39883700	-0.00120100	0.00064800
C	-5.71089900	-1.12577500	0.46040400
C	-4.31251300	-1.13441800	0.46477700
C	-3.46943100	2.26071800	-0.95208400
C	-3.16690200	2.34541500	-2.32830900
C	-2.24960600	3.30011400	-2.75985500
C	-1.61796500	4.17400700	-1.86897400

C	-1.94168200	4.08307500	-0.51769600
C	-2.85506100	3.13685700	-0.03593300
C	-3.76501800	1.37229000	-3.30209200
C	-0.58621200	5.14715700	-2.35835700
C	-3.12969500	3.06301600	1.44090100
C	-3.46828800	-2.26209100	0.95241800
C	-3.16534300	-2.34678400	2.32856500
C	-2.24742200	-3.30103200	2.75974200
C	-1.61559500	-4.17454500	1.86859400
C	-1.93972700	-4.08362200	0.51743000
C	-2.85370200	-3.13778400	0.03601900
C	-3.76362600	-1.37404300	3.30262800
C	-0.58320700	-5.14719600	2.35763100
C	-3.12867200	-3.06388200	-1.44075000
C	3.63715600	0.00055800	-0.00002500
C	4.31258600	1.13420500	0.46443600
C	5.71095700	1.12541500	0.46000000
C	6.39876500	0.00073200	0.00026900
C	5.71120900	-1.12400600	-0.45961900
C	4.31280300	-1.13297100	-0.46436600
C	3.46849700	2.26197600	0.95207900
C	3.16585000	2.34692300	2.32826200
C	2.24807200	3.30131100	2.75947800
C	1.61611900	4.17470500	1.86832600
C	1.93996400	4.08353300	0.51709600
C	2.85378000	3.13757900	0.03565100
C	3.76430700	1.37435300	3.30238700
C	0.58394200	5.14756500	2.35739800
C	3.12855700	3.06350100	-1.44114400
C	3.46913000	-2.26092600	-0.95231700
C	2.85519100	-3.13739400	-0.03620100
C	1.94190600	-4.08370600	-0.51792700
C	1.61778900	-4.17436000	-1.86913600
C	2.24897300	-3.30011000	-2.75998700
C	3.16621300	-2.34533500	-2.32846700
C	3.13007800	-3.06357200	1.44057500
C	0.58602600	-5.14753700	-2.35843900
C	3.76383000	-1.37184200	-3.30219300
H	-6.26109300	1.99955400	-0.81353900
H	-7.49167200	-0.00138500	0.00081500
H	-6.26016900	-2.00192500	0.81476300
H	-2.00237500	3.34909300	-3.82413200
H	-1.46252500	4.75982900	0.19467200
H	-3.41260500	0.34821700	-3.09427200

H	-3.48286000	1.62145100	-4.33389100
H	-4.86269000	1.34556000	-3.23613100
H	0.37557000	4.63427200	-2.52650300
H	-0.41234800	5.95353900	-1.63154800
H	-0.88147300	5.60451900	-3.31434400
H	-4.09392500	2.58507700	1.65939200
H	-3.12945800	4.06823200	1.88720500
H	-2.34515000	2.48081100	1.95666800
H	-1.99983500	-3.35000400	3.82393900
H	-1.46045200	-4.76005400	-0.19516200
H	-4.86129600	-1.34745800	3.23669200
H	-3.41134500	-0.34985200	3.09511200
H	-3.48141400	-1.62345600	4.33435100
H	-0.87794900	-5.60472300	3.31370200
H	0.37835200	-4.63381800	2.52547600
H	-0.40916200	-5.95348500	1.63076100
H	-4.09313100	-2.58627800	-1.65900800
H	-3.12814600	-4.06904100	-1.88718400
H	-2.34444900	-2.48133900	-1.95658500
H	6.26035300	2.00152500	0.81427000
H	7.49159900	0.00081600	0.00040200
H	6.26075500	-2.00004500	-0.81382700
H	2.00075800	3.35047100	3.82372800
H	1.46056900	4.75989100	-0.19548600
H	3.41214600	0.35009900	3.09499000
H	3.48213300	1.62385000	4.33409900
H	4.86197600	1.34788100	3.23638000
H	-0.37759400	4.63431800	2.52576300
H	0.40969800	5.95362800	1.63032900
H	0.87904100	5.60538600	3.31322000
H	4.09306300	2.58602400	-1.65944900
H	3.12781700	4.06860400	-1.88770400
H	2.34434900	2.48077900	-1.95681500
H	1.46312300	-4.76075700	0.19441300
H	2.00143100	-3.34886800	-3.82420300
H	3.12823700	-4.06863000	1.88721600
H	2.34654100	-2.47991800	1.95622400
H	4.09509500	-2.58710100	1.65884100
H	0.41230200	-5.95400100	-1.63168300
H	0.88114900	-5.60479500	-3.31452600
H	-0.37579800	-4.63466900	-2.52638500
H	3.48167800	-1.62099800	-4.33399500
H	4.86149300	-1.34465400	-3.23632600
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3.3.3. $[TerSnAs]_4$

0 1

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Sn	-0.04185500	1.81383200	-1.10797100
As	-2.35755300	0.83907400	-0.17629400
As	0.08529800	-2.04320000	1.34491400
As	0.79240500	-0.42560000	-2.33000000
As	1.47205300	1.72818300	1.08383700
C	-1.52898800	0.95740000	3.83194600
C	-2.29970400	0.01025900	4.53549000
C	-2.63252600	0.24629900	5.87555800
C	-2.23579800	1.41858600	6.51009300
C	-1.56640900	2.39613900	5.78277300
C	-1.22630300	2.19276200	4.43683800
C	-2.89721700	-1.19114100	3.88300300
C	-2.39666400	-2.47957900	4.14166700
C	-3.05713600	-3.58801500	3.60982200
C	-4.19058500	-3.45645900	2.80666400
C	-4.68436500	-2.17056100	2.58339400
C	-4.06833500	-1.03426500	3.11209600
C	-1.15378800	-2.65541000	4.95707100
C	-4.83890000	-4.64863700	2.16753200
C	-4.68121900	0.31755300	2.88631400
C	-0.70243200	3.39267300	3.71585600
C	0.59829800	3.86953900	3.95856100
C	0.97291600	5.12468000	3.47360100
C	0.08078300	5.93560400	2.77244300
C	-1.19133000	5.42710000	2.50630100
C	-1.60105900	4.16958100	2.95419500
C	1.56625100	3.04090200	4.74403300
C	0.44867400	7.32445900	2.33876300
C	-2.99312000	3.69737000	2.64833700
C	-2.45688800	-3.18503500	-1.51897600
C	-2.00370200	-4.48548900	-1.19161000
C	-2.87788400	-5.57698600	-1.27882800
C	-4.18622200	-5.41540400	-1.71436000
C	-4.60449500	-4.15790900	-2.12111600
C	-3.75696100	-3.03808000	-2.04291300
C	-0.58988800	-4.85744200	-0.88849400
C	-0.22795200	-5.34166300	0.38311300
C	1.05004900	-5.86727100	0.57534100
C	1.97555600	-5.95692800	-0.46481800

C	1.57577400	-5.52399700	-1.72887000
C	0.31652200	-4.96644400	-1.96181800
C	-1.20992700	-5.33845600	1.51246200
C	3.36239300	-6.47353900	-0.22430100
C	-0.07590000	-4.55564200	-3.35241800
C	-4.35354300	-1.83227500	-2.69625800
C	-3.97549300	-1.52126800	-4.01677600
C	-4.79976800	-0.68614800	-4.77946200
C	-5.98502900	-0.15199100	-4.27486600
C	-6.30953700	-0.42785800	-2.94355500
C	-5.50700600	-1.23804400	-2.14174000
C	-2.73810000	-2.10684600	-4.63335800
C	-6.84379700	0.75811200	-5.10145800
C	-5.85633300	-1.46091700	-0.70141300
C	3.91937300	-1.77362600	0.19893600
C	4.20561000	-2.27489200	1.48906900
C	5.20413300	-3.24060300	1.66663500
C	5.92168400	-3.72643400	0.58126600
C	5.69772800	-3.17795600	-0.67497000
C	4.73603200	-2.17598900	-0.88091600
C	3.55203500	-1.74078600	2.71703400
C	2.76010500	-2.57522000	3.53168200
C	2.23917300	-2.06579000	4.72138700
C	2.46840700	-0.75137200	5.13025900
C	3.30185600	0.03885700	4.33656100
C	3.85453400	-0.42968400	3.14187200
C	2.48268400	-3.99980900	3.15307700
C	1.81392600	-0.20811300	6.36599800
C	4.80342500	0.44821000	2.37660600
C	4.81780200	-1.51895900	-2.22328000
C	5.88846400	-0.62192000	-2.42858000
C	6.11620200	-0.11068700	-3.70746700
C	5.31305400	-0.45882200	-4.79618000
C	4.27283300	-1.35981300	-4.57504600
C	4.02701800	-1.91136500	-3.31353000
C	6.80885000	-0.25301500	-1.30005800
C	5.54009400	0.14833300	-6.14885200
C	3.01359200	-2.99774200	-3.16565900
C	0.12652500	3.61658200	-2.33015800
C	1.40203900	4.14522100	-2.59480300
C	1.54203300	5.17060400	-3.53963700
C	0.43357400	5.69142900	-4.19822500
C	-0.83648600	5.22489800	-3.87496900
C	-1.00040000	4.20038500	-2.93612300

C	2.61659200	3.74610700	-1.82955900
C	3.51167200	2.78429900	-2.32017600
C	4.70228900	2.55503700	-1.62154400
C	5.02680600	3.25562600	-0.45932100
C	4.10223500	4.18278800	0.02628500
C	2.90486000	4.44304600	-0.63816600
C	3.24093600	2.04472300	-3.59799100
C	6.33566600	3.03639200	0.24370900
C	1.94208200	5.44410000	-0.07976400
C	-2.36836000	3.81211200	-2.50896100
C	-3.01834400	2.70742600	-3.07903600
C	-4.27155600	2.34119100	-2.58813300
C	-4.89283700	3.04437800	-1.55296900
C	-4.23903800	4.15640000	-1.02396500
C	-2.98394300	4.55664400	-1.48700500
C	-2.35405400	1.90683600	-4.16134600
C	-6.20027200	2.57865600	-0.98447100
C	-2.30197100	5.75754600	-0.89857400
H	-3.23096200	-0.49691500	6.40927000
H	-2.49156000	1.59162800	7.55823600
H	-1.32508500	3.35722700	6.24459700
H	-2.66819600	-4.58548300	3.82832900
H	-5.59986900	-2.04750000	2.00040700
H	-0.88230200	-3.71659000	5.04675500
H	-1.25662300	-2.23604400	5.96946100
H	-0.31460800	-2.12982400	4.47780100
H	-4.61325300	-5.57573600	2.71396200
H	-4.47437200	-4.77772600	1.13395300
H	-5.93193900	-4.53519700	2.11534300
H	-5.67920800	0.22449100	2.43607600
H	-4.06775300	0.92970500	2.20685400
H	-4.77369300	0.87981600	3.82767200
H	1.98656500	5.48567300	3.67161000
H	-1.90610000	6.04371700	1.95670100
H	1.29216100	2.99238200	5.80994300
H	2.58547100	3.44537100	4.67056200
H	1.57822100	2.00822200	4.36960900
H	0.20260800	7.49491000	1.27956600
H	1.52095500	7.52209900	2.47557100
H	-0.10554800	8.07573100	2.92485600
H	-2.99378800	2.95107900	1.83555000
H	-3.62505300	4.53249500	2.31680400
H	-3.46602300	3.22322900	3.51977700
H	-2.49892100	-6.57036200	-1.02567000

H	-4.86138000	-6.27197500	-1.77897800
H	-5.60528000	-4.02129700	-2.53879400
H	1.32257300	-6.23531800	1.56810500
H	2.26244400	-5.63965700	-2.57013100
H	-1.82178600	-4.42778700	1.50948100
H	-0.69301800	-5.39471900	2.48043200
H	-1.90091100	-6.19582200	1.44828600
H	3.37675300	-7.25089600	0.55377200
H	4.02142700	-5.65581000	0.11303800
H	3.80354300	-6.89193600	-1.14059500
H	-1.05975500	-4.96504900	-3.62623200
H	0.66240400	-4.90425700	-4.08698000
H	-0.15054400	-3.46042700	-3.44633900
H	-4.51615400	-0.47233900	-5.81441800
H	-7.21687100	0.00444800	-2.51294900
H	-2.70343900	-3.19942200	-4.51080600
H	-1.82564400	-1.70692300	-4.16066000
H	-2.68441100	-1.87390300	-5.70552200
H	-6.67869200	0.60556600	-6.17745600
H	-6.61253900	1.81428300	-4.87888600
H	-7.91290000	0.60721400	-4.89101500
H	-5.92910300	-2.52873200	-0.44893100
H	-6.80638100	-0.97459900	-0.43945300
H	-5.06597400	-1.04012800	-0.05923800
H	5.41800400	-3.59867800	2.67657200
H	6.68229600	-4.49862000	0.71950300
H	6.30433900	-3.49542800	-1.52756900
H	1.63554400	-2.72219600	5.35230400
H	3.55585200	1.04864100	4.66513700
H	1.56162700	-4.35680900	3.63535900
H	3.30365200	-4.66799900	3.46224100
H	2.36182300	-4.11080400	2.06789800
H	0.80090400	0.16459300	6.13427600
H	2.38180900	0.63095100	6.79235400
H	1.70622200	-0.98309100	7.13905200
H	5.71133600	-0.10327100	2.08886000
H	5.09781500	1.31740100	2.98036800
H	4.35162100	0.83675500	1.44997000
H	6.94827100	0.58433800	-3.85676400
H	3.63752300	-1.66346700	-5.41214300
H	6.24642000	0.01393300	-0.39442800
H	7.45414400	0.59295800	-1.57422400
H	7.45937400	-1.09772300	-1.02444800
H	6.60408600	0.36688300	-6.32115700

H	4.99086700	1.10017700	-6.24524100
H	5.18868700	-0.51346200	-6.95344900
H	2.25383600	-2.94793600	-3.95556400
H	2.50455700	-2.97568900	-2.19359600
H	3.51307300	-3.97786100	-3.23312300
H	2.54149300	5.56605300	-3.73873500
H	0.55717300	6.48308600	-4.94128500
H	-1.72447900	5.66055100	-4.34066500
H	5.40421600	1.82924400	-2.03133800
H	4.32582500	4.73510800	0.94366300
H	3.46254300	0.97446300	-3.49095400
H	3.87852600	2.42761600	-4.41203000
H	2.19700300	2.14821200	-3.92070500
H	6.34804500	2.08141200	0.79074300
H	6.53499800	3.83528300	0.97193300
H	7.17323300	3.00927300	-0.46936200
H	1.59146600	6.15090000	-0.84622100
H	2.40213200	6.01062700	0.73929500
H	1.05062400	4.94143700	0.33056700
H	-4.75748600	1.45895000	-3.00100300
H	-4.71324200	4.72601100	-0.21915500
H	-3.07032200	1.23466900	-4.64923300
H	-1.54262900	1.27589300	-3.75691700
H	-1.89152000	2.55484400	-4.92000800
H	-6.93307300	2.35885200	-1.77492500
H	-6.63694900	3.32859000	-0.30973800
H	-6.05555900	1.65036800	-0.40659100
H	-2.92983000	6.22661500	-0.12892400
H	-2.08140200	6.51294800	-1.66794200
H	-1.33720700	5.48770400	-0.44201500

3.3.4. TerSnP

0 1

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C	-1.22692600	-1.68856700	-0.00009900
C	-1.21087900	-3.08691800	-0.00022400
C	0.00006100	-3.77795700	-0.00027500
C	1.21098000	-3.08688500	-0.00022900
C	1.22698300	-1.68853500	-0.00012100
C	-2.48952000	-0.90024900	-0.00006600
C	-3.06462600	-0.50311500	-1.22299900
C	-4.20273700	0.30438900	-1.19858200

C	-4.78215400	0.72669200	-0.00003200
C	-4.20299200	0.30399600	1.19848100
C	-3.06485900	-0.50350900	1.22286500
C	-2.45584800	-0.92779000	-2.52877600
C	-5.97314100	1.63936900	-0.00005700
C	-2.45634100	-0.92854700	2.52864500
C	2.48955400	-0.90018400	-0.00009800
C	3.06488900	-0.50344700	1.22285600
C	4.20299200	0.30407100	1.19847700
C	4.78216400	0.72678400	-0.00004700
C	4.20277900	0.30446800	-1.19858900
C	3.06466500	-0.50305800	-1.22300800
C	2.45641700	-0.92861500	2.52861400
C	5.97311800	1.63950000	0.00000600
C	2.45593600	-0.92778000	-2.52879600
H	-2.15868600	-3.63115600	-0.00027400
H	0.00007300	-4.87059100	-0.00036300
H	2.15880600	-3.63109000	-0.00028600
H	-4.64631800	0.61916300	-2.14762700
H	-4.64676500	0.61845400	2.14754000
H	-1.43110500	-0.53753100	-2.64101500
H	-3.04872100	-0.56444800	-3.37882200
H	-2.37970600	-2.02347800	-2.60128800
H	-6.59832000	1.48808600	-0.89177600
H	-5.65166000	2.69421200	0.00065400
H	-6.59910800	1.48712800	0.89094400
H	-2.37994400	-2.02423500	2.60076500
H	-3.04953400	-0.56566800	3.37867100
H	-1.43173100	-0.53805300	2.64131600
H	4.64676100	0.61856700	2.14752700
H	4.64634400	0.61925500	-2.14763400
H	2.38158000	-2.02438500	2.60128500
H	1.43119500	-0.53957700	2.64064700
H	3.04876000	-0.56446400	3.37868500
H	6.59871400	1.48771300	0.89134800
H	5.65158700	2.69432800	0.00007900
H	6.59869900	1.48784000	-0.89137300
H	2.38055600	-2.02350900	-2.60159400
H	3.04841000	-0.56380800	-3.37884800
H	1.43089700	-0.53823400	-2.64073900

3.3.5. $[TerSnP]_2$

0 1

Sn	-1.45287100	0.17453000	-0.02697500
Sn	1.45289800	-0.17457300	-0.02739600
P	-0.00025400	-0.00010200	-1.99694600
P	0.00031000	0.00022900	1.93978600
C	-3.57488300	0.47025100	0.05677700
C	-4.06901400	1.71170000	-0.36042100
C	-5.44366800	1.94744300	-0.27027200
C	-6.28740600	0.95227500	0.22721200
C	-5.78015800	-0.28198700	0.63744700
C	-4.40661300	-0.53535200	0.55771800
C	-3.05906900	2.66607400	-0.90095600
C	-2.83052700	2.69528200	-2.29429600
C	-1.74998400	3.42263400	-2.78487300
C	-0.88150400	4.11803700	-1.93749700
C	-1.13871500	4.09696000	-0.56955800
C	-2.21349800	3.37984700	-0.02732600
C	-3.68485100	1.88459200	-3.22475900
C	0.32476500	4.81509700	-2.49200300
C	-2.41283300	3.37685200	1.46411800
C	-3.75557400	-1.80695300	0.98122800
C	-3.35726900	-1.96784000	2.32496300
C	-2.62958100	-3.10149200	2.68055400
C	-2.28680200	-4.08208000	1.74552000
C	-2.69621400	-3.90531000	0.42482300
C	-3.41906000	-2.77788000	0.01879400
C	-3.64637000	-0.90081200	3.33932200
C	-1.47700400	-5.27635200	2.15878700
C	-3.79019000	-2.60519400	-1.42784500
C	3.57491200	-0.47021400	0.05664200
C	4.40658900	0.53538400	0.55765400
C	5.78012600	0.28200400	0.63759100
C	6.28741900	-0.95227900	0.22748700
C	5.44372400	-1.94747000	-0.27003800
C	4.06909100	-1.71169700	-0.36040200
C	3.75553800	1.80700000	0.98112000
C	3.35747600	1.96801700	2.32492300
C	2.62971900	3.10160800	2.68052100
C	2.28659700	4.08203100	1.74542800
C	2.69577800	3.90514900	0.42468700
C	3.41870000	2.77775500	0.01864100
C	3.64681700	0.90110800	3.33934000
C	1.47668100	5.27622300	2.15869000
C	3.78944300	2.60501800	-1.42809800
C	3.05922700	-2.66613400	-0.90096900

C	2.21365300	-3.37992500	-0.02734900
C	1.13886200	-4.09700800	-0.56958700
C	0.88163400	-4.11803900	-1.93752900
C	1.75015100	-3.42268900	-2.78489700
C	2.83070100	-2.69533900	-2.29430600
C	2.41295100	-3.37688900	1.46409400
C	-0.32476700	-4.81490300	-2.49199100
C	3.68496400	-1.88458500	-3.22477000
H	-5.85232500	2.91087600	-0.58578600
H	-7.36133700	1.14235400	0.29657200
H	-6.45180400	-1.05410500	1.02169700
H	-1.55825900	3.42076500	-3.86151000
H	-0.47497100	4.63796000	0.10931500
H	-3.55132300	0.80680800	-3.03422500
H	-3.41889600	2.07657700	-4.27294900
H	-4.75600000	2.09582400	-3.09133400
H	0.12838100	5.23537600	-3.48909200
H	1.15727400	4.09919800	-2.59506600
H	0.66253500	5.62942700	-1.83507900
H	-3.40704100	3.00830500	1.74875500
H	-2.29114500	4.39236000	1.87008300
H	-1.66060000	2.73674400	1.95941100
H	-2.30496300	-3.21374500	3.71895300
H	-2.44168900	-4.66317200	-0.32059600
H	-4.70552300	-0.60468700	3.33511300
H	-3.05963600	0.00713800	3.12075200
H	-3.37830600	-1.23365100	4.35100400
H	-1.92024100	-5.78086500	3.03121500
H	-0.45604000	-4.97537500	2.44557900
H	-1.39627100	-6.01237100	1.34640300
H	-4.77949600	-2.14132500	-1.54584700
H	-3.79109100	-3.57175800	-1.95090500
H	-3.06495100	-1.95429900	-1.94737200
H	6.45170700	1.05414200	1.02191400
H	7.36134100	-1.14236600	0.29698000
H	5.85239700	-2.91093300	-0.58544300
H	2.30531600	3.21394700	3.71897700
H	2.44103500	4.66290300	-0.32076400
H	3.05994300	-0.00682000	3.12101900
H	3.37905200	1.23408200	4.35105500
H	4.70593700	0.60489100	3.33487700
H	0.45584000	4.97510200	2.44577500
H	1.39561800	6.01208200	1.34619900
H	1.92001500	5.78097000	3.03093600

H	4.77798400	2.13962300	-1.54639000
H	3.79181900	3.57178500	-1.95079000
H	3.06306500	1.95550600	-1.94777900
H	0.47509400	-4.63797700	0.10929100
H	1.55842700	-3.42081700	-3.86153400
H	2.29095800	-4.39233000	1.87013500
H	1.66087500	-2.73652100	1.95928600
H	3.40724600	-3.00858700	1.74874800
H	-0.66216900	-5.62972600	-1.83547700
H	-0.12876900	-5.23446400	-3.48945500
H	-1.15739200	-4.09902500	-2.59418100
H	3.41949500	-2.07711200	-4.27298500
H	4.75617300	-2.09517300	-3.09086200
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3.3.6. $[TerSnP]_4$

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Sn	0.84124200	-0.23347800	1.84373500
Sn	0.89295700	1.52511000	-0.98770800
Sn	-2.03745100	0.34550700	0.16674800
Sn	0.24311800	-1.84197300	-0.98892900
P	2.31382600	-0.49639500	-0.24146500
P	-0.32506700	1.95874300	1.20635200
P	-0.92069700	0.13508200	-2.15469200
P	-1.09497700	-1.81220000	1.22658900
C	1.84244400	-0.49242600	3.74844000
C	2.47919300	0.60219600	4.37831400
C	2.88467900	0.46850600	5.71238400
C	2.70564900	-0.72467100	6.40239100
C	2.20697400	-1.83735900	5.73692000
C	1.80699100	-1.74517700	4.39713200
C	2.91006600	1.83714500	3.65603200
C	2.29315900	3.08404000	3.88322500
C	2.80921000	4.22026000	3.26391100
C	3.91356100	4.17174800	2.41055000
C	4.53268700	2.93809800	2.22955200
C	4.05555600	1.77204200	2.83726100
C	1.06136300	3.20285900	4.72545800
C	4.38406100	5.39354600	1.68016200
C	4.80796700	0.49724900	2.60359200
C	1.52938900	-3.03421700	3.68477600
C	0.35323900	-3.75472400	3.94452400
C	0.20642300	-5.04374700	3.42413300
C	1.20334400	-5.65257300	2.66784500

C	2.35941800	-4.91460900	2.40403300
C	2.54953900	-3.62547700	2.90228000
C	-0.74850500	-3.15891000	4.76283200
C	1.05103600	-7.06501800	2.18627700
C	3.85597600	-2.94832700	2.62724900
C	1.83659500	3.35128300	-1.71718900
C	1.24115200	4.58603200	-1.36287300
C	1.96949800	5.77317000	-1.50330300
C	3.26136600	5.77563500	-2.01324200
C	3.80367000	4.58341300	-2.46178600
C	3.10499400	3.36784500	-2.34026300
C	-0.19759700	4.79341200	-1.01324700
C	-0.59070100	5.19386600	0.27091100
C	-1.92364700	5.54041200	0.49995400
C	-2.88008600	5.53070700	-0.51465800
C	-2.44954100	5.20971500	-1.80151000
C	-1.13367200	4.82874400	-2.07256500
C	0.40922900	5.30546800	1.37619300
C	-4.31984800	5.80596100	-0.20436700
C	-0.72962300	4.51136100	-3.48271300
C	3.78102600	2.26017400	-3.09226300
C	3.32978600	1.96557600	-4.39491500
C	4.15283100	1.23514400	-5.25450000
C	5.41756400	0.78931900	-4.87045900
C	5.82230000	1.03952500	-3.55903400
C	5.01962600	1.74034200	-2.65720700
C	2.00466300	2.45919700	-4.89318100
C	6.28265900	-0.00409100	-5.80358300
C	5.44788800	1.87623200	-1.22853300
C	-4.06411600	1.18219000	0.38914800
C	-4.34592800	1.67685500	1.68249200
C	-5.44532600	2.51979700	1.89445300
C	-6.26080600	2.90154600	0.83453900
C	-6.02352000	2.35634300	-0.41970900
C	-4.96481000	1.46203200	-0.65594300
C	-3.56497200	1.27773500	2.89037100
C	-2.84332600	2.24746800	3.61700100
C	-2.15430100	1.85920500	4.76463300
C	-2.15643400	0.54060700	5.22108200
C	-2.94336100	-0.38718300	4.53182800
C	-3.64864500	-0.04786400	3.37296900
C	-2.82533000	3.68070300	3.17742700
C	-1.31709600	0.13954900	6.39718200
C	-4.49976400	-1.07721600	2.68719300

C	-5.01968800	0.79374200	-1.99382400
C	-6.03595100	-0.16535100	-2.18528300
C	-6.24337500	-0.70187100	-3.45391700
C	-5.47242900	-0.31569300	-4.55505900
C	-4.49089700	0.64990500	-4.35159400
C	-4.25798100	1.22323500	-3.09401000
C	-6.92811000	-0.57521400	-1.04693500
C	-5.67112200	-0.95581000	-5.89717300
C	-3.29113100	2.35985900	-2.98797600
C	0.20544300	-3.70003200	-2.12728200
C	-1.01793800	-4.36504000	-2.33568400
C	-1.07857900	-5.42298200	-3.25152000
C	0.05875800	-5.84351700	-3.93111400
C	1.28031200	-5.23638600	-3.66160600
C	1.36665300	-4.16865100	-2.76233200
C	-2.23353400	-4.05881000	-1.53233200
C	-3.26142500	-3.22549300	-2.02327100
C	-4.42569200	-3.08913400	-1.27246700
C	-4.62057900	-3.77196000	-0.06911900
C	-3.57661200	-4.55533700	0.41512000
C	-2.38207100	-4.71187500	-0.29706700
C	-3.15698600	-2.52604800	-3.34946800
C	-5.95341500	-3.72154200	0.62436000
C	-1.28819500	-5.57369500	0.25107200
C	2.69742900	-3.63692800	-2.38002600
C	3.15968200	-2.42989400	-2.91568400
C	4.37406700	-1.91599900	-2.46098500
C	5.13880400	-2.57428100	-1.49583800
C	4.67368300	-3.79333900	-1.00143900
C	3.46647800	-4.34324300	-1.43460400
C	2.35268000	-1.66666100	-3.92029300
C	6.40330100	-1.96004300	-0.97258600
C	2.99208500	-5.67377900	-0.92288200
H	3.37142400	1.31503900	6.20235200
H	3.02008500	-0.80029800	7.44589300
H	2.15390100	-2.81072100	6.22943800
H	2.32757800	5.18368200	3.44821200
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H	0.81301900	4.25489300	4.92801000
H	1.14599500	2.67626400	5.68599800
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H	5.47761100	5.39996500	1.56444400

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H	4.28175400	-0.13561600	1.86983800
H	4.91511200	-0.09884900	3.51900300
H	-0.71250000	-5.59734500	3.63350100
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H	-1.64788900	-3.79111500	4.73151500
H	-1.02198300	-2.18474700	4.33796100
H	1.16231400	-7.14036300	1.09319000
H	0.06903500	-7.47531700	2.45492400
H	1.82060300	-7.71828600	2.62796100
H	3.75774400	-2.18510000	1.83884000
H	4.59889300	-3.67810200	2.27829300
H	4.25335100	-2.44657600	3.51954000
H	1.48694600	6.71396900	-1.22678800
H	3.81635800	6.71137600	-2.10857700
H	4.78177800	4.56382400	-2.94683600
H	-2.21378400	5.84065600	1.50984100
H	-3.16062900	5.26379100	-2.62869600
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H	-4.43154800	6.51600100	0.62835400
H	-4.80892800	4.87085200	0.11825200
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H	3.80052600	1.02584200	-6.26825100
H	6.79222300	0.66407300	-3.22068700
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H	1.89489000	2.27136700	-5.96955800
H	6.03449300	0.19574000	-6.85585800
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H	7.34807600	0.22402000	-5.65484500
H	5.46588400	2.92193700	-0.89624600
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H	-5.64674700	2.87271500	2.90807400
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H	-6.69200400	2.59068100	-1.25203600
H	-1.61003000	2.61174600	5.33818700
H	-3.02539800	-1.40555900	4.91721100

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H	-3.73448400	4.22406900	3.48035900
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H	-3.88894800	0.98994200	-5.19912200
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H	-7.47554500	-1.49856500	-1.28364300
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H	-2.03791400	-5.92088100	-3.41185900
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H	-3.69556500	-5.06404000	1.37462300
H	-3.19893800	-1.43376800	-3.20989300
H	-3.98461500	-2.80443600	-4.02091300
H	-2.22178500	-2.75284500	-3.87538100
H	-6.24797600	-2.70053500	0.89231900
H	-5.97090400	-4.33735000	1.53205700
H	-6.72861800	-4.12109500	-0.05204900
H	-0.88920900	-6.26223700	-0.50884200
H	-1.64797300	-6.16699600	1.10257600
H	-0.44588200	-4.96202300	0.61155200
H	4.72676700	-0.96392200	-2.85515000
H	5.26526100	-4.33311800	-0.25596900
H	3.00832400	-1.12732500	-4.61443300
H	1.72146100	-0.90094100	-3.43667300
H	1.67526300	-2.31260000	-4.49513400
H	7.06873800	-1.64451000	-1.79123500
H	6.95852500	-2.66110000	-0.33507000
H	6.17883100	-1.05787500	-0.38034400
H	3.68559800	-6.08750300	-0.17750800
H	2.92176100	-6.40234700	-1.74498600

H 1.99121900 -5.60475400 -0.47258700

4. References

[1] G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw, K. I. Goldberg, *Organometallics* **2010**, *29*, 2176–2179.

[2] R. S. Simons, L. Pu, M. M. Olmstead, P. P. Power, *Organometallics* **1997**, *16*, 1920–1925.

[3] D. Heift, Z. Benkő, H. Grützmacher, *Dalton Trans.* **2014**, *43*, 831–840.

[4] A. Doddi, M. Weinhart, A. Hinz, D. Bockfeld, J. M. Goicoechea, M. Tamm, *Chem. Commun.* **2017**, *7*, 6069–6072.

[5] A. Hinz, J. M. Goicoechea, *Angew. Chem. Int. Ed.* **2016**, *55*, 8536–8541.

[6] J. Cosier, A. M. Glazer, *J. Appl. Cryst.* **1986**, *19*, 105.

[7] CrysAlisPro, Agilent Technologies, Version 1.171.35.8.

[8] G. M. Sheldrick, **2013**, SHELXS-2013.

[9] C. B. Hübschle, G. M. Sheldrick, B. Dittrich, *J. Appl. Crystallogr.* **2011**, *44*, 1281–1284.

[10] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, *Gaussian 09, revision D.01*, Gaussian, Inc., Wallingford CT, **2009**..

[11] E. D. Glendening, C. R. Landis, F. Weinhold, *J. Comput. Chem.* **2013**, *34*, 1429–1437.

[12] a) G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders, T. Ziegler, *J. Comput. Chem.* **2001**, *22*, 931; b) C. Fonseca Guerra, J. G. Snijders,

G. te Velde, E. J. Baerends, *Theor. Chem. Acc.* **1998**, *99*, 391; c) ADF2013.01, SCM, Theoretical Chemistry, Vrije Universiteit: Amsterdam, The Netherlands, http://www.scm.com.

[13] a) E. van Lenthe, E. J. Baerends, J. G. Snijders, *J. Chem. Phys.* **1993**, *99*, 4597; b) E. van Lenthe, E. J. Baerends, J. G. Snijders, *J. Chem. Phys.* **1994**, *101*, 9783; c) E. van Lenthe, A. Ehlers, E. J. Baerends, *J. Chem. Phys.* **1999**, *110*, 8943