Electronic Supplementary Information for

Transformation of Nortricyclane Type Cage Compounds Cage Compounds E_4Q_3 (E = P, Q = S, Se; E = As, Q = S) by $[Cp''_2Zr(CO)_2]$

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1. Experimental details

All manipulations were performed under an atmosphere of dry nitrogen and under exclusion of oxygen and moisture using standard Schlenk and glovebox techniques. All solvents were dried using conventional techniques, degassed and saturated with nitrogen prior to use. ^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H}, ^{31}P and ^{77}Se NMR spectra were recorded on a Bruker Avance 400 (^{1}H: 400.130 MHz, ^{13}C: 100.613 MHz, ^{31}P: 161.976 MHz, ^{77}Se: 76.299 MHz) or on a Bruker Avance 300 (^{1}H: 300.132 MHz, ^{13}C: 75.468 MHz, ^{31}P: 121.495 MHz). The chemical shifts are reported in ppm relative to external TMS (^{1}H, ^{13}C), external Me_2Se (^{77}Se) and H_3PO_4 (85%) (^{31}P). Mass spectrometry was performed using a Finnigan MAT95 LIFDI-MS and a Joel AccuTOF GC X and using a Finnigan SSQ 710 A (EI). IR spectra were recorded on a Bruker ALPHA device with a diamond ATR unit. [Cp"$_2$Zr(CO)$_2$] and E_4Q_3 were prepared according to literature.[1] Due to the intense air and moisture sensitivity of the phosphorus containing products as well as the fractional crystallization no satisfying elemental analysis could be performed of the latter.

Synthesis of [(Cp"$_2$Zr)$_2$(μ,η$^{1:1:1:1}$-P$_2$S$_4$)] (1)

To a boiling solution of P_4S_3 (112 mg, 0.509 mmol) in 30 mL toluene a solution of [Cp"$_2$Zr(CO)$_2$] (500 mg, 0.996 mmol) in 60 mL toluene was added dropwise within 20 min. After refluxing the purple solution for additionally 1 h, all volatiles were removed in *vacuo*. The brown-purple solid was slurried in *n*-hexane (30 mL) and filtered over a plug of diatomaceous earth. **1** can be isolated by fractional crystallization. Crystals of [(Cp"$_2$Zr)$_2$(μ,η$^{1:1:1:1}$-P$_2$S$_4$)] suitable for a single crystal X-ray diffraction were obtained by storage of a concentrated *n*-hexane solution at -30°C. Crystalline Yield: 81 mg (30 % based on P_4S_3, overall yield 60% as determined by ^{31}P NMR spectroscopy of the crude reaction mixture). ^{1}H NMR (C_6D_6, 400 MHz, 300 K): δ [ppm] = 1.29 (s, 36 H, C(CH_3)$_3$), 1.41 (s, 36 H, C(CH_3)$_3$), 5.61 (d, ^{4}J(H,H) = 2.6 Hz, 4 H, C$_5H_3$*t*Bu$_2$), 5.79 (d, ^{4}J(H,H) = 2.6 Hz, 4 H, C$_5H_3$*t*Bu$_2$), 5.80 (t, ^{4}J(H,H) = 2.6 Hz, 2 H, C$_5H_3$*t*Bu$_2$), 5.96 (t, br, ^{4}J(H,H) = 2.6 Hz, 2 H, C$_5H_3$*t*Bu$_2$); ^{13}C{^{1}H} NMR (C_6D_6, 100 MHz, 300 K): δ [ppm] = 31.4 (s, C(*C*H$_3$)$_3$), 32.6 (s, C(*C*H$_3$)$_3$), 34.3 (s, *C*(CH$_3$)$_3$), 34.5 (s, *C*(CH$_3$)$_3$), 104.5 (s, *C*$_5$H$_3$*t*Bu$_2$), 104.8 (s, *C*$_5$H$_3$*t*Bu$_2$), 112.1 (s, *C*$_5$H$_3$*t*Bu$_2$), 115.4 (s, br, *C*$_5$H$_3$*t*Bu$_2$), 146.3 (s, *C*$_5$H$_3$*t*Bu$_2$), 147.1 (s, *C*$_5$H$_3$*t*Bu$_2$); ^{31}P{^{1}H} NMR (C_6D_6, 161 MHz, 300 K): δ [ppm] = -24.3 (s, *P*$_2$S$_4$); ^{31}P NMR (C_6D_6, 161 MHz, 300 K): δ [ppm] = -24.3 (s, *P*$_2$S$_4$); FD-MS (toluene): *m/z* [%] = 1080.38 (100) [M$^{+\cdot}$]; elemental analysis: [$C_{52}H_{84}Zr_2P_2S_4$] calc.: C, 57.73; H, 7.83; S, 11.85. found: C, 54.21; H, 7.23; S, 9.13; despite several attempts, even by using Sn capsules, no satisfying elemental analysis could be obtained due to the air and moisture sensitivity of the compound. Interestingly, the found data fit nicely the oxidation product [Cp"$_2$Zr(PS$_2$O$_2$)] (calc.: C, 54.51; H, 7.39; S, 11.19).

Synthesis of [(Cp"$_2$Zr)$_2$(μ,η$^{1:1:1:1}$-P$_2$Se$_4$)] (2)

To a boiling solution of P_4Se_3 (180 mg, 0.499 mmol) in 40 mL toluene a solution of [Cp"$_2$Zr(CO)$_2$] (500 mg, 0.996 mmol) in 60 mL toluene was added dropwise within 25 min. After refluxing the purple solution for additionally 1.25 h, all volatiles were removed in *vacuo*. The darkpurple solid was slurried in *n*-hexane (30 mL), stirred overnight and filtered over a plug of diatomaceous earth. Crystals of [(Cp"$_2$Zr)$_2$(μ,η$^{1:1:1:1}$-P$_2$Se$_4$)] suitable for a single crystal X-ray diffraction were obtained by storage of a concentrated *n*-hexane solution at -30°C. Crystalline Yield: 72 mg (23 % based on P_4Se_3, overall yield 85% as determined by ^{31}P NMR spectroscopy of the crude reaction mixture). ^{1}H NMR (C_6D_6, 400 MHz, 300 K): δ [ppm] = 1.28 (s, 36 H, C(CH_3)$_3$), 1.42 (s, 36 H, C(CH_3)$_3$), 5.50 (d, ^{4}J(H,H) = 2.6 Hz, 4 H, C$_5H_3$*t*Bu$_2$), 5.66 (d, ^{4}J(H,H) = 2.6 Hz, 4 H, C$_5H_3$*t*Bu$_2$), 5.86 (m, asymmetric superposition, 4 H, C$_5H_3$*t*Bu$_2$); ^{13}C{^{1}H} NMR (C_6D_6, 100 MHz, 300 K): δ [ppm] = 31.6 (s, C(*C*H$_3$)$_3$), 32.7 (s, C(*C*H$_3$)$_3$), 34.4 (s, *C*(CH$_3$)$_3$), 34.6 (s, *C*(CH$_3$)$_3$), 104.1 (s, *C*$_5$H$_3$*t*Bu$_2$), 104.1 (s, *C*$_5$H$_3$*t*Bu$_2$), 112.0 (s, *C*$_5$H$_3$*t*Bu$_2$), 115.7 (s, br, *C*$_5$H$_3$*t*Bu$_2$), 146.2 (s, *C*$_5$H$_3$*t*Bu$_2$), 147.2 (s, *C*$_5$H$_3$*t*Bu$_2$); ^{31}P{^{1}H} NMR (C_6D_6, 161 MHz, 300 K): δ [ppm] = -47.9 (s, *P*$_2$Se$_4$); ^{31}P NMR (C_6D_6, 161 MHz, 300 K): δ [ppm] = -47.9 (s, *P*$_2$Se$_4$); ^{77}Se NMR (C_6D_6, 76 MHz, 300 K): δ [ppm] = 323.2 (pt, P$_2$Se$_4$); FD-MS (toluene): *m/z* [%] = 1268.16 (100) [M$^{+\cdot}$]; elemental analysis: [$C_{52}H_{84}Zr_2P_2Se_4$] calc.: C, 49.20; H, 6.67. found: C, 45.67; H, 6.02; despite several

attempts, even by using Sn capsules, no satisfying elemental analysis could be obtained due to the air and moisture sensitivity of the compound. Interestingly, the found data fit nicely the oxidation product [Cp"$_2$Zr(PSe_2O_2)] (calc.: C, 46.84; H, 6.35).

Synthesis of [(Cp"$_2$Zr)$_2$(μ,η$^{1:1:1:1}$-As_2S_4)] (3)

To a boiling solution of As_4S_3 (201 mg, 0.508 mmol) in 30 mL toluene a solution of [Cp"$_2$Zr(CO)$_2$] (500 mg, 0.996 mmol) in 70 mL toluene was added dropwise within 15 min. After refluxing the purple solution for additionally 1 h, all volatiles were removed in *vacuo*. The red purple solid was slurried in *n*-hexane (30 mL), stirred overnight and filtered over a plug of diatomaceous earth. Crystals of [(Cp"$_2$Zr)$_2$(μ,η$^{1:1:1:1}$-As_2S_4)] suitable for a single crystal X-ray diffraction were obtained by storage of a concentrated toluene solution at -30°C. Crystalline Yield: 60 mg (21 % based on As_4S_3). ^{1}H NMR (C_6D_6, 400 MHz, 300 K): δ [ppm] = 1.32 (s, 36 H, C(CH_3)$_3$), 1.38 (s, 36 H, C(CH_3)$_3$), 5.59 (d, ^4J(H,H) = 2.6 Hz, 4 H, C_5H_3tBu$_2$), 5.72 (d, ^4J(H,H) = 2.6 Hz, 4 H, C_5H_3tBu$_2$), 5.82 (t, ^4J(H,H) = 2.6 Hz, 2 H, C_5H_3tBu$_2$), 5.85 (t, br, ^4J(H,H) = 2.6 Hz, 2 H, C_5H_3tBu$_2$); ^{13}C{^{1}H} NMR (C_6D_6, 100 MHz, 300 K): δ [ppm] = 31.4 (s, C(CH$_3$)$_3$), 32.4 (s, C(CH$_3$)$_3$), 34.3 (s, C(CH$_3$)$_3$), 34.5 (s, C(CH$_3$)$_3$), 104.1 (s, C_5H$_3t$Bu$_2$), 104.3 (s, C_5H$_3t$Bu$_2$), 109.7 (s, C_5H$_3t$Bu$_2$), 112.8 (s, br, C_5H$_3t$Bu$_2$), 146.3 (s, C_5H$_3t$Bu$_2$), 146.4 (s, C_5H$_3t$Bu$_2$); FD-MS (toluene): *m/z* [%] = 1168.26 (51) [M$^{+\cdot}$], 583.13 (100) [½M$^{+\cdot}$]; elemental analysis: [$C_{52}H_{84}Zr_2As_2S_4$] calc.: C, 53.39; H, 7.24; S, 10.96. found: C, 53.40; H, 7.11; S, 10.79.

2. Simulation of the NMR spectra of 2

The ^{31}P and ^{77}Se NMR spectra were simulated with the WIN-DAISY module in Topspin 3.0 processing software (Bruker-Franzen GmbH)[2]. Table S1 and Table S2 show the determined parameters: chemical shift (δ), linewidth ($\omega_{1/2}$) and the coupling constants (*J*) for the simulation of the phosphorus and selenium NMR spectra, respectively. The ratio between the non, the mono and the bis ^{77}Se substituted isomers was defined by the natural abundance of ^{77}Se (7.63%). The isomers with three and four ^{77}Se nuclei were not taken into account due to their low natural abundance.

Table S1. Linewidth, chemical shifts and coupling constants obtained from the simulation of the ^{31}P NMR spectrum of **2**. Only the non and the mono ^{77}Se substituted isomers were used for the simulation.

δ [ppm]	Number of ^{77}Se atoms	P1	P1'
	0	-47.88	-
	1	-47.88	-47.87
$\omega_{1/2}$ [Hz]	0	8.00	-
	1	10.24	10.24
J [Hz]		P1'	Se1
	P1	^{1}J = 248.38	^{1}J = -210.99
	P1'	-	^{2}J = 28.0731

Table S2. Linewidth, chemical shifts and coupling constants obtained from the simulation of the ^{77}Se NMR spectrum of **2**. Only the mono and the bis ^{77}Se substituted isomers (cis, trans and geminal) were used for the simulation.

δ [ppm]	Number of ^{77}Se atoms	Se1	Se2	
	1	323.18	-	
	2 (cis)	323.17	323.18	
	2 (trans)	323.18	323.18	
	2 (geminal)	323.18	323.18	
$\omega_{1/2}$ [Hz]				
	1	10.2438	-	
	2 (cis)	2.6261	2.6261	
	2 (trans)	3.6373	3.6373	
	2 (geminal)	3.7598	3.7598	
J [Hz]	cis	Se2	P1	P1'
	Se1	^{3}J = 28.8088	^{1}J = -210.09	^{2}J = 15.6371
	Se2	-	^{2}J = 28.1086	^{1}J = -211.14
	P1	-	-	^{1}J = 263.04
J [Hz]	trans	Se2	P1	P1'
	Se1	^{3}J = 51.9751	^{1}J = -205.61	^{2}J = 27.3147
	Se2	-	^{2}J = 20.3724	^{1}J = -204.51
	P1	-	-	^{1}J = 284.26
J [Hz]	geminal	Se2	P1	P1'
	Se1	^{2}J = 39.9442	^{1}J = -212.95	^{2}J = 28.9658
	Se2	-	^{1}J = -215.75	^{2}J = 29.0817
	P1	-	-	^{1}J = 211.94

3. NMR spectra of compounds 1, 2 and 3

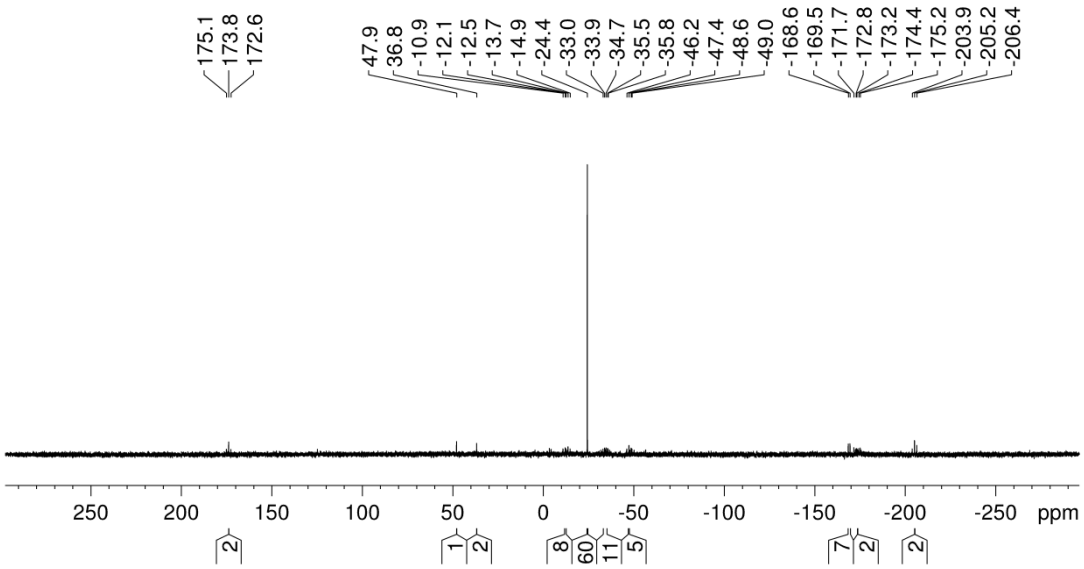

Fig. S1 ^{31}P NMR spectrum of the crude reaction mixture of **1** in C_6D_6.

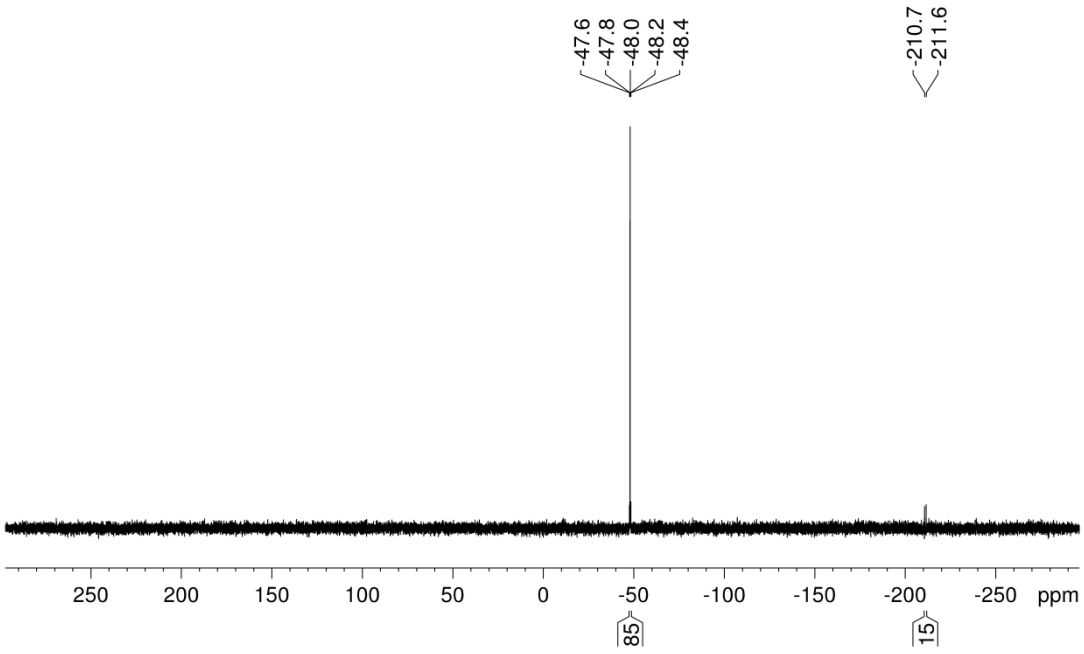

Fig. S2 ^{31}P NMR spectrum of the crude reaction mixture of **2** in C_6D_6.

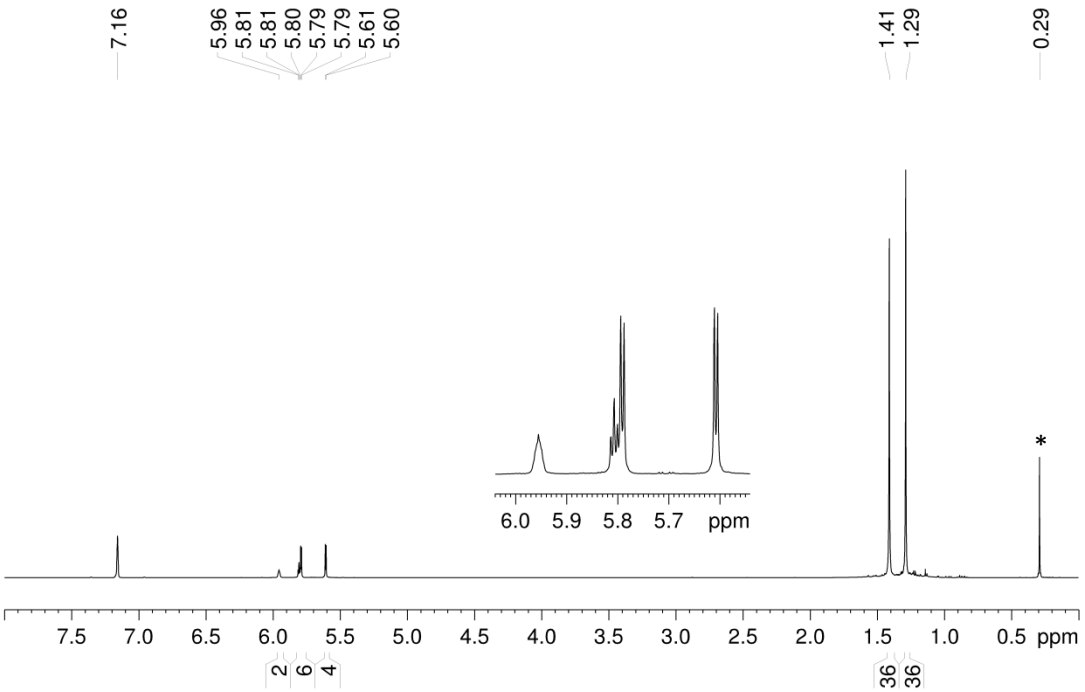

Fig. S3 ^{1}H NMR spectrum of crystalline **1** in C_6D_6. The signal marked with * is due to silicon grease.

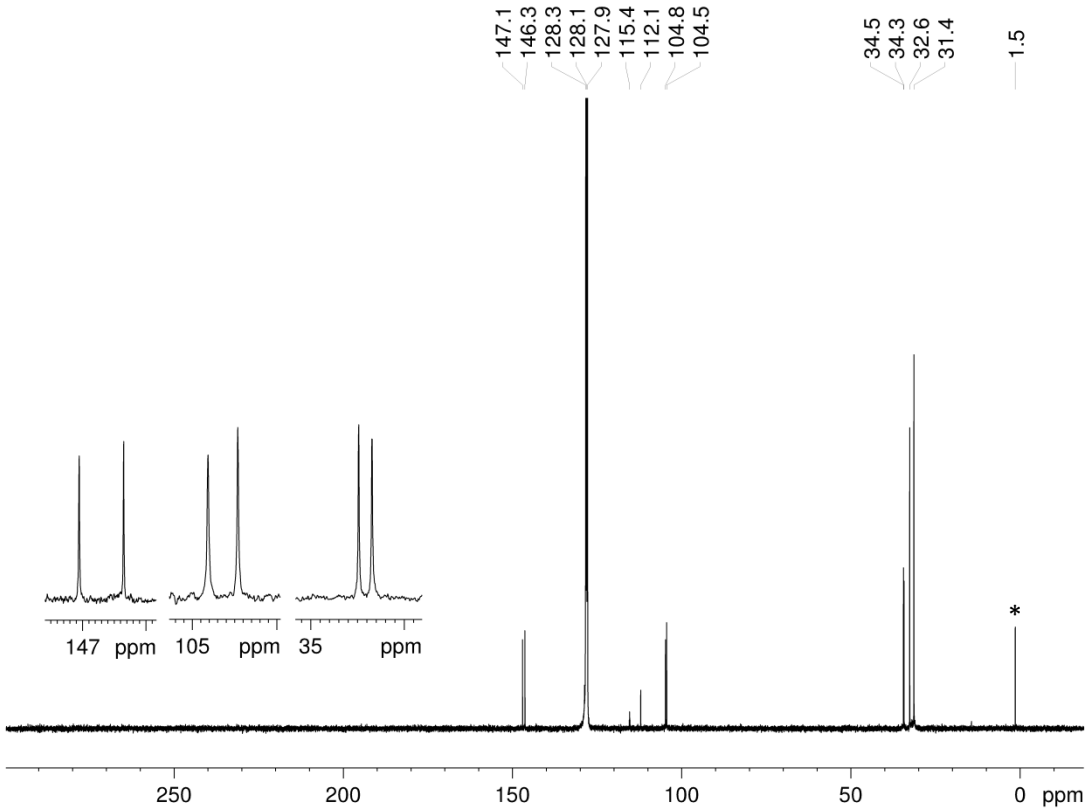

Fig. S4 $^{13}C\{^{1}H\}$ NMR spectrum of crystalline **1** in C_6D_6. The signal marked with * is due to silicon grease.

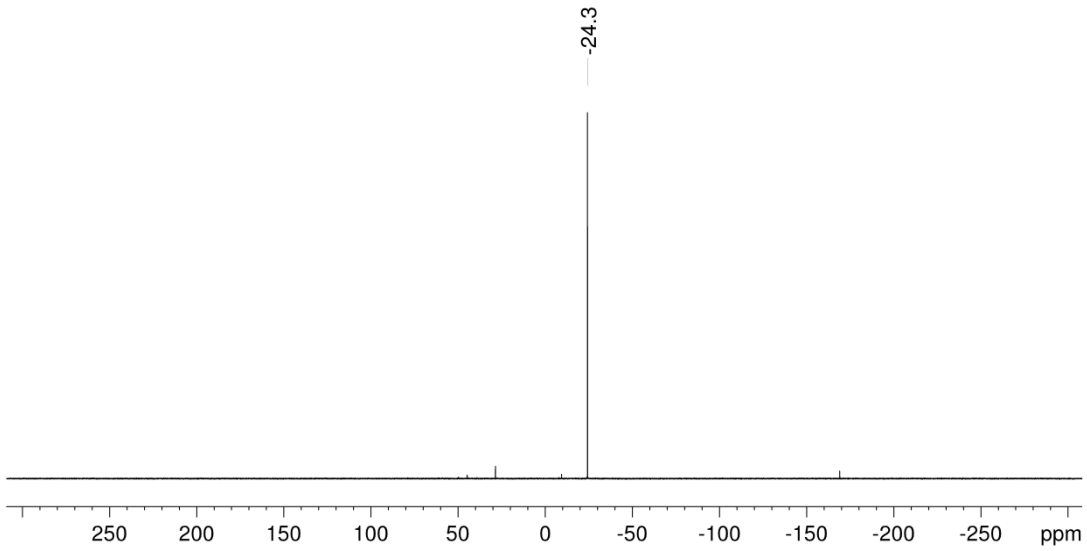

Fig. S5 $^{31}P\{^{1}H\}$ NMR spectrum of crystalline **1** in C_6D_6.

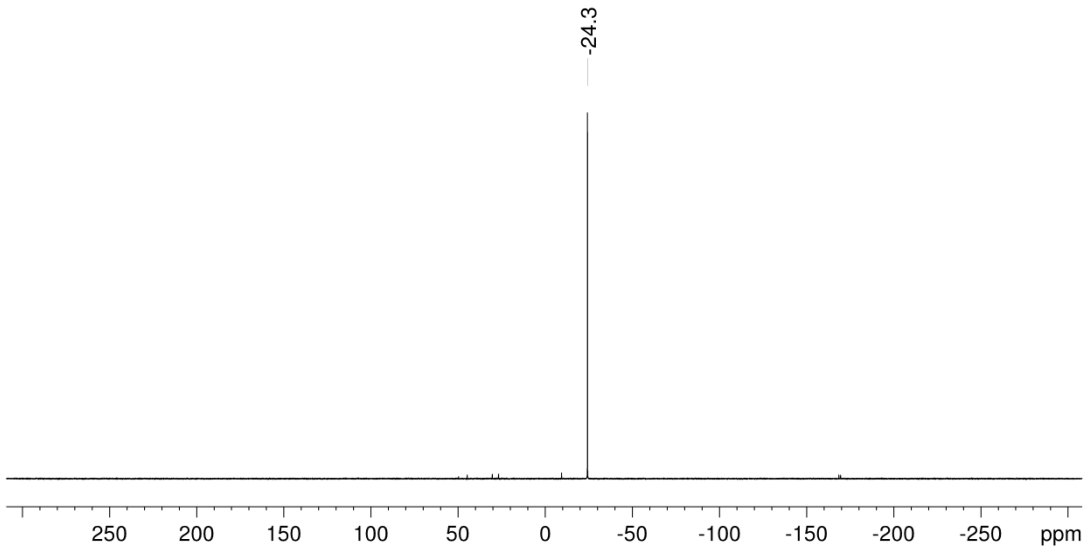

Fig. S6 ^{31}P NMR spectrum of crystalline **1** in C_6D_6.

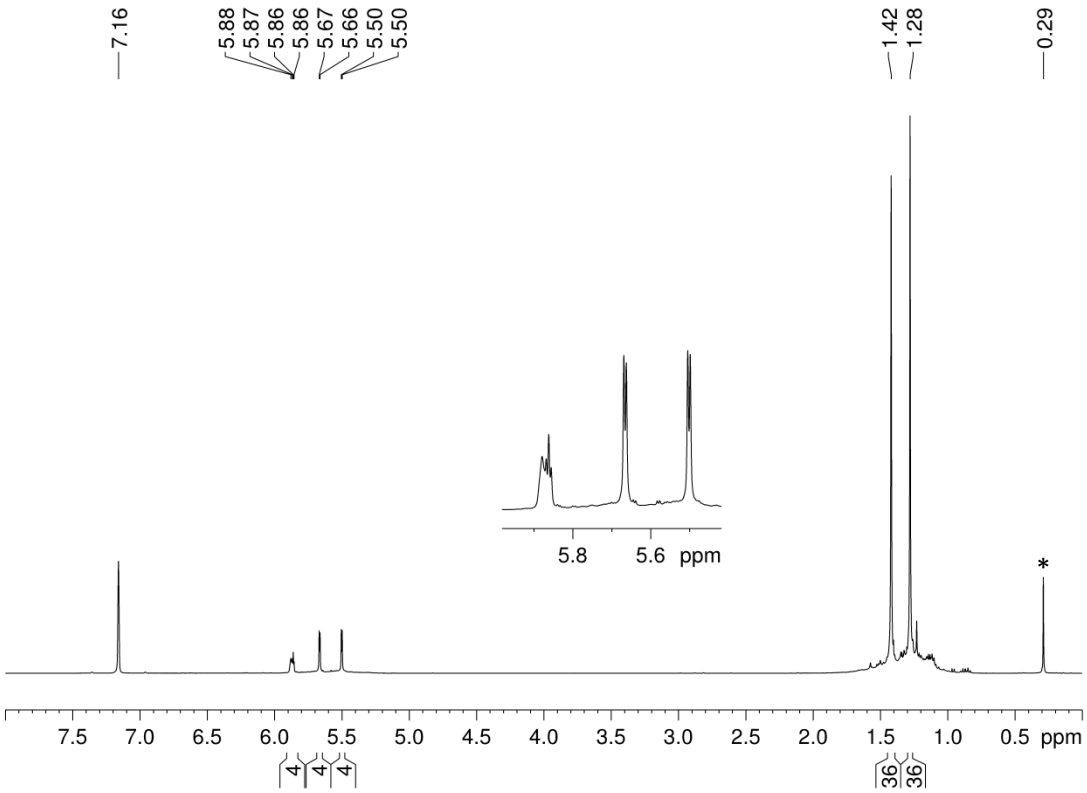

Fig. S7 ^{1}H NMR spectrum of crystalline **2** in C_6D_6. The signal marked with * is due to silicon grease.

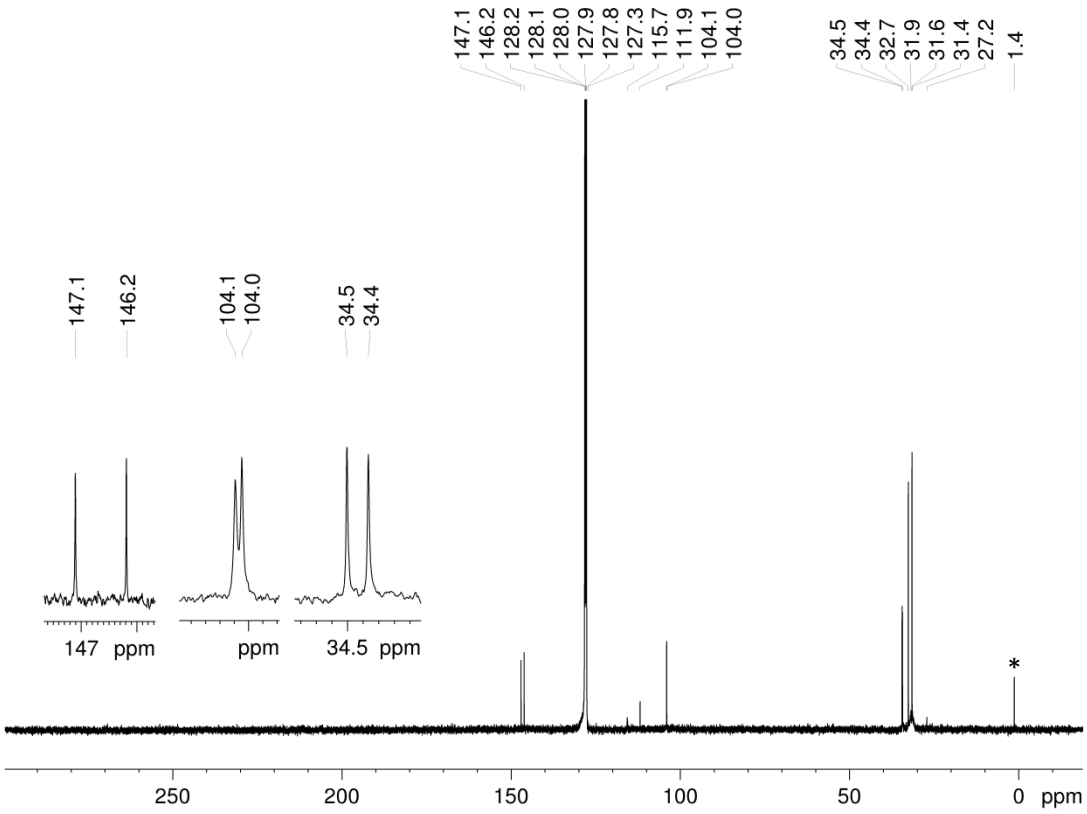

Fig. S8 $^{13}C\{^{1}H\}$ NMR spectrum of crystalline **2** in C_6D_6. The signal marked with * is due to silicon grease.

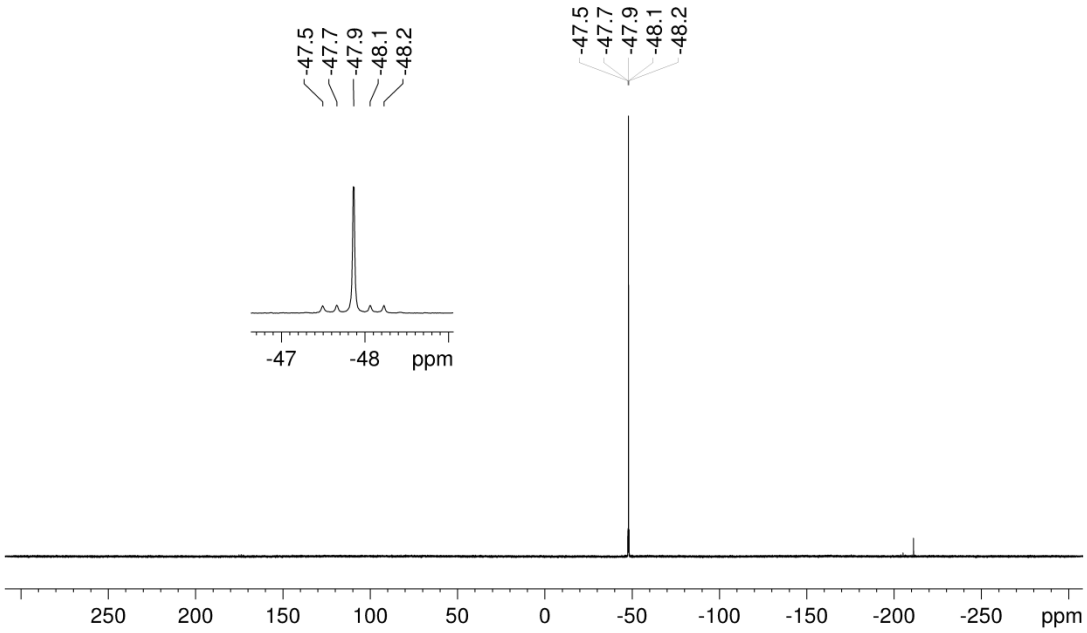

Fig. S9 $^{31}P\{^{1}H\}$ NMR spectrum of crystalline **2** in C_6D_6.

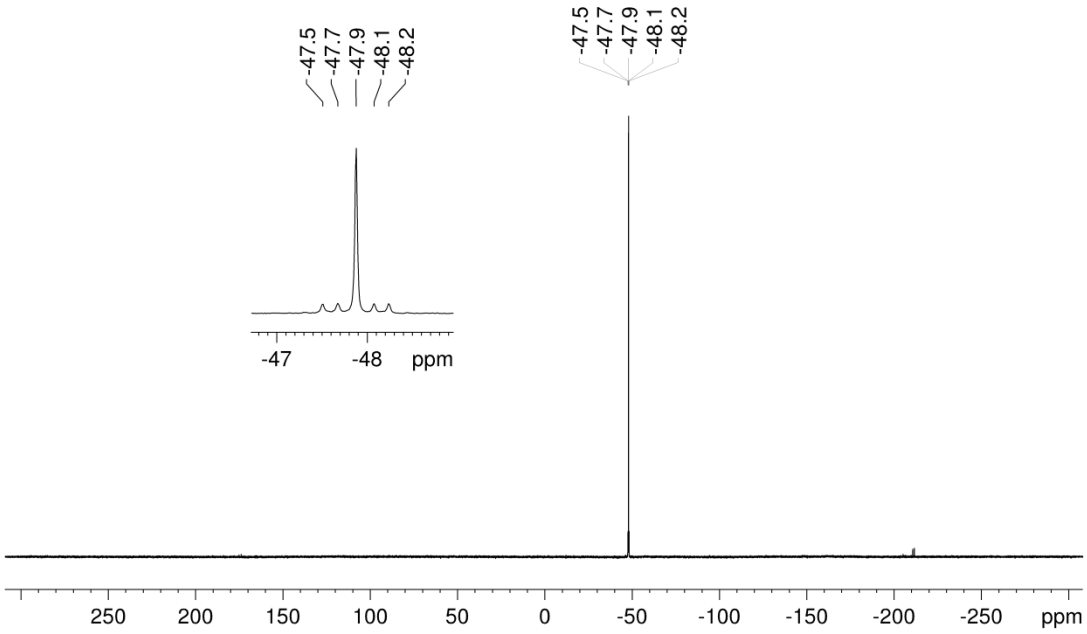

Fig. S10 ^{31}P NMR spectrum of crystalline **2** in C_6D_6.

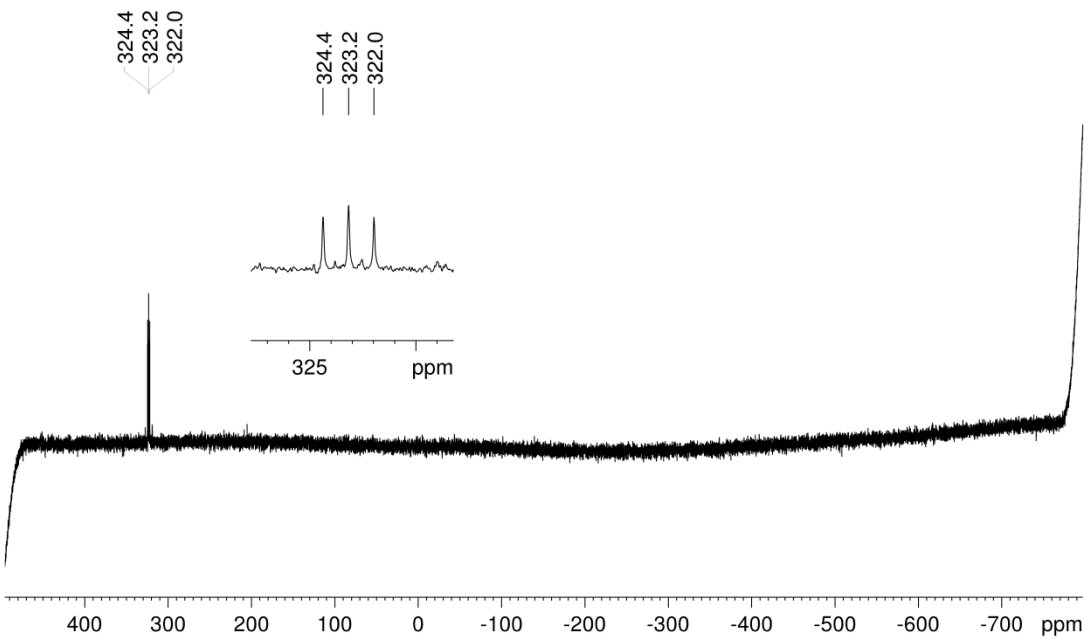

Fig. S11 ^{77}Se NMR spectrum of crystalline **2** in C_6D_6.

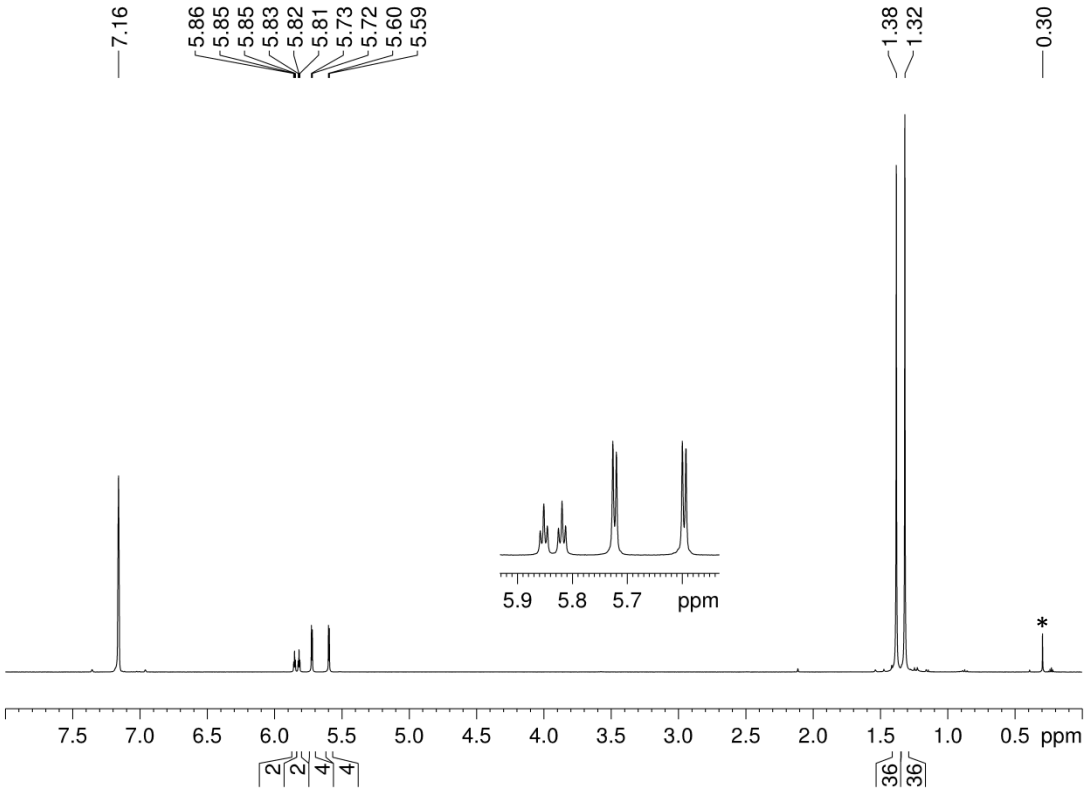

Fig. S12 ^{1}H NMR spectrum of crystalline **3** in C_6D_6. The signal marked with * is due to silicon grease.

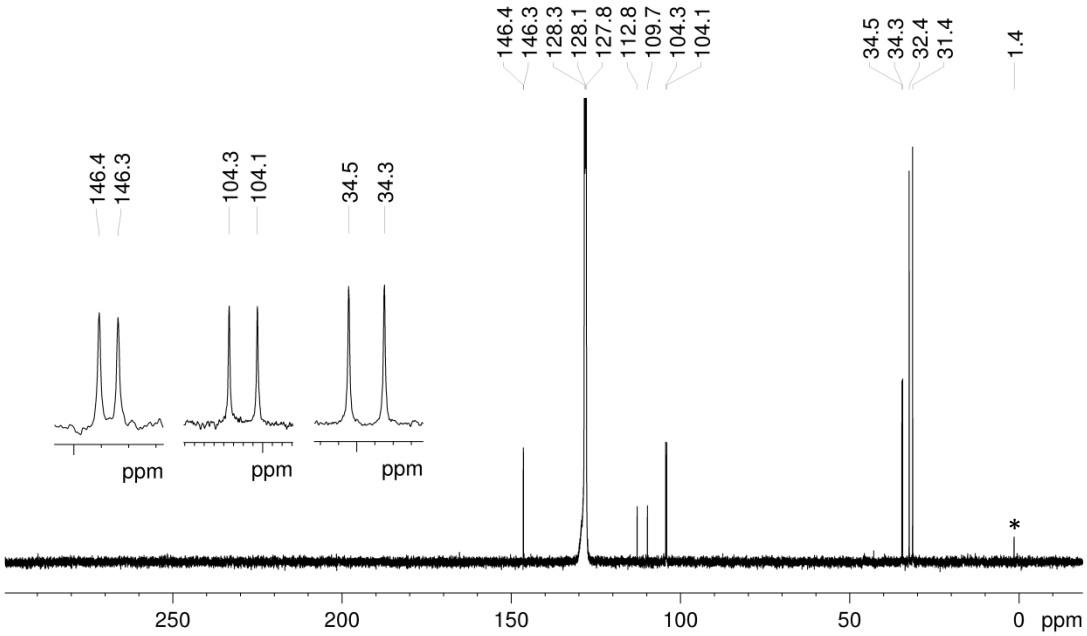

Fig. S13 $^{13}C\{^{1}H\}$ NMR spectrum of crystalline **3** in C_6D_6. The signal marked with * is due to silicon grease.

4. Crystallographic data

Suitable single crystals were measured on a GV50, Titan[S2] diffractometer with $Cu_{K\alpha}$ radiation. Frames integration and data reduction were performed with the CrysAlisPro ver. 171.37.34 software package.[3] Using Olex2[4], the structures were solved with the ShelXT[5] structure solution program using Direct Methods and refined with the ShelXL[5] refinement package using Least Squares minimisation. Further details are given in Table S3. The pictures of the molecular structures were created using Olex2[4].

CCDC reference number CCDC-1518491 (**1**), -1518492 (**2**) and -1518493 (**3**) contain the supplementary crystallographic data for **1**, **2** and **3**, respectively. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retreving.html or from the Cambridge Crystallographic Data Center, 12 union Road, Cambridge CB2 1EZ, UK; Fax: (internat.) +44-1223-336-033; E-mail: deposit@ccdc.cam.ac.uk

Table S3. Structure determination summary of complexes **1**, **2** and **3**.

Compound	**1**	**2**	**3** · 2 C_7H_8
Empirical formula	$C_{52}H_{84}P_2S_4Zr_2$	$C_{52}H_{84}P_2Se_4Zr_2$	$C_{80}H_{116}As_2S_4Zr_2$
Formula weight	1081.81	1269.41	1538.24
Temperature/K	123(1)	123(1)	123(1)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	C2/c	P21/n	P21/n
a/Å	24.7202(5)	15.2831(3)	12.6043(2)
b/Å	13.6790(2)	9.91947(18)	12.6538(2)
c/Å	16.2972(3)	18.6250(3)	24.3651(4)
α/°	90	90	90
β/°	95.8930(16)	102.8354(18)	95.3864(15)
γ/°	90	90	90
Volume/Å^3	5481.75(17)	2753.00(9)	3868.89(11)
Z	4	2	2
ρcalcg/cm^3	1.311	1.531	1.320
μ/mm^{-1}	5.325	6.908	4.463
F(000)	2280.0	1284.0	1612.0
Crystal size/mm^3	0.2127 × 0.1206 × 0.0323	0.0857 × 0.0662 × 0.0517	0.1288 × 0.0947 × 0.0554
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.19 to 134.142	6.786 to 134.118	7.288 to 134.068
Index ranges	-26 ≤ h ≤ 29, -13 ≤ k ≤ 16, -19 ≤ l ≤ 19	-13 ≤ h ≤ 18, -11 ≤ k ≤ 11, -19 ≤ l ≤ 22	-11 ≤ h ≤ 15, -15 ≤ k ≤ 14, -29 ≤ l ≤ 23
Reflections collected	14672	10319	13931
Independent reflections	4884 [Rint = 0.0473, Rsigma = 0.0421]	4872 [Rint = 0.0707, Rsigma = 0.0767]	6855 [Rint = 0.0322, Rsigma = 0.0422]
Data/restraints/parameters	4884/0/283	4872/0/283	6855/0/411
Goodness-of-fit on F^2	1.055	1.021	1.021
Final R indexes [I>=2σ (I)]	R1 = 0.0344, wR2 = 0.0883	R1 = 0.0518, wR2 = 0.1236	R1 = 0.0334, wR2 = 0.0779
Final R indexes [all data]	R1 = 0.0397, wR2 = 0.0941	R1 = 0.0624, wR2 = 0.1327	R1 = 0.0444, wR2 = 0.0842
Largest diff. peak/hole / e Å^{-3}	0.86/-0.59	1.76/-1.22	0.80/-0.42

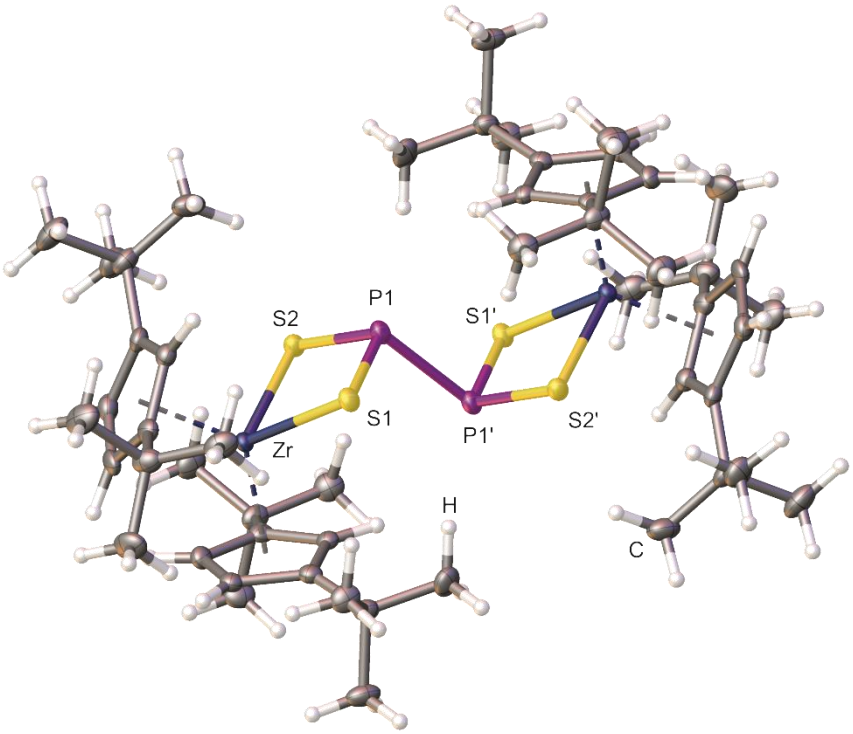

Fig. S14 Grown molecular structure of **1** in the solid state. The ellipsoids are drawn at the 50% probability level. Selected bond lengths [Å] and angles [°]: S2-P1 2.1139(10), S1-P1 2.1133(9), P1-P1' 2.2593(14), S2-P1-P1' 102.19(5), S1-P1-S2 106.06(4), S1-P1-P1' 99.56(5).

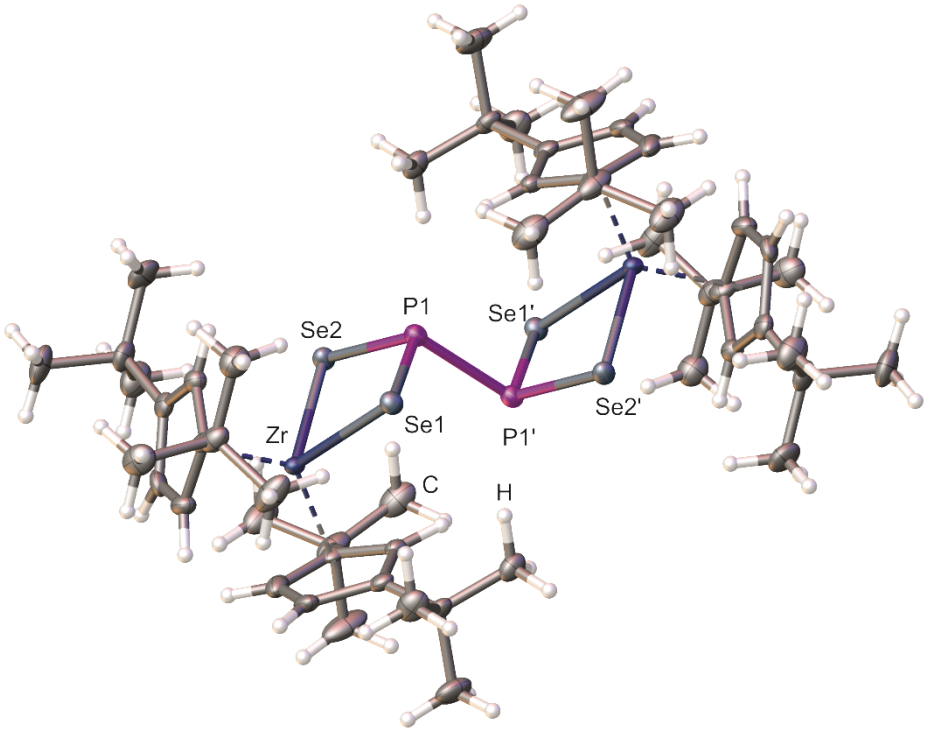

Fig. S15 Grown molecular structure of **2** in the solid state. The ellipsoids are drawn at the 50% probability level. Selected bond lengths [Å] and angles [°]: Se2-P1 2.2515(15), Se1-P1 2.2538(14), P1-P1' 2.266(3), Se2-P1-Se1 106.40(5), Se2-P1-P1' 101.91(9), Se1-P1-P1' 103.04(8).

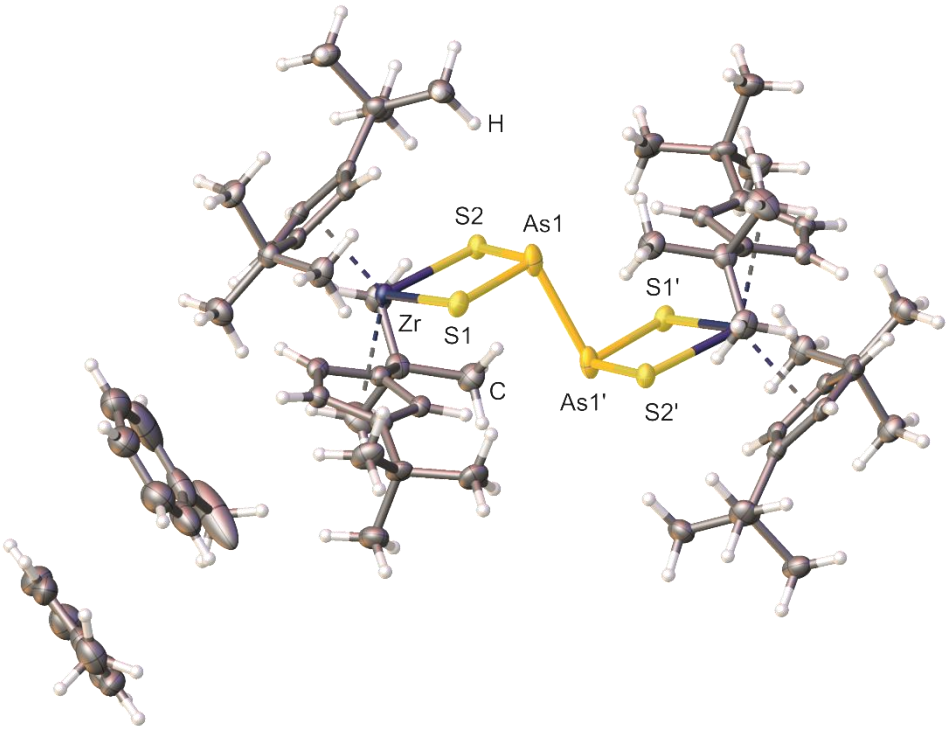

Fig. S16 Grown asymmetric unit of **3** in the solid state. The ellipsoids are drawn at the 50% probability level. Two molecules of toluene are co crystallized. Selected bond lengths [Å] and angles [°]: As1-As1’ 2.4876(8), As1-S1 2.2376(7), As1-S2 2.2343(8), S1-As1-As1’ 95.53(3), S2-As1-As1’ 98.85(3), S2-As1-S1 102.22(3).

5. Computational details

The geometries of the compounds have been fully optimized with gradient-corrected density functional theory (DFT) in form of Becke's three-parameter hybrid method B3LYP[7] with def2-SVP all electron basis set (ECP for Zr).[8] Gaussian 09 program package[9] was used throughout. All structures correspond to minima on their respective potential energy surfaces. Since it was shown that the extended basis set is required to adequately reproduce the relative energies of $C_2S_2H_2$ isomers,[10] for the computations of the relative energies of $(HQ)_2EE(QH)_2$ and (HQ)(Q)HEEH(Q)(QH) isomers all electron def2-TZVPPD basis set[11] (def2-TZVPP basis set of Ahlrichs[8a] with additional diffuse functions) was also employed. Basis sets were obtained from the EMSL basis set exchange database.[12] For the estimation of planarization energies of P and As centers in **1**-**4** the optimization was performed with one Q_2EE moiety constrained to be planar.

Table S4. Reaction energies $\Delta E°_0$, standard enthalpies $\Delta H°_{298}$, Gibbs energies $\Delta G°_{298}$ (kJ mol^{-1}) and standard entropies $\Delta S°_{298}$ (J mol^{-1} K^{-1}) for the considered gas phase processes. B3LYP/def2-SVP level of theory.

Process	$\Delta E°_0$	$\Delta H°_{298}$	$\Delta S°_{298}$	$\Delta G°_{298}$	$\Delta G°_{384}$
$2Cp''_2Zr(CO)_2 + 2\ P_4S_3 =$ **1** $+ 2\ CO + ¼\ S_8 + {}^3/_2\ P_4$	65.0	53.7	396.2	-64.4	-98.3
$2Cp''_2Zr(CO)_2 + 2\ P_4Se_3 =$ **2** $+ 2\ CO + ¼\ Se_8 + {}^3/_2\ P_4$	84.0	73.7	388.9	-42.3	-75.5
$2Cp''_2Zr(CO)_2 + 2\ As_4S_3 =$ **3** $+ 2\ CO + ¼\ S_8 + {}^3/_2\ As_4$	70.6	59.0	389.6	-57.1	-90.4
$2Cp''_2Zr(CO)_2 + 2\ As_4Se_3 =$ **4** $+ 2\ CO + ¼\ Se_8 + {}^3/_2\ As_4$	118.8	107.2	379.3	-5.8	-38.3
$2P_4S_3 = 2P_4 + {}^3/_4S_8$	348.0	343.4	142.8	300.9	288.6
$2P_4Se_3 = 2P_4 + {}^3/_4Se_8$	201.1	198.1	145.2	154.8	142.3
$2As_4S_3 = 2As_4 + {}^3/_4S_8$	357.5	353.3	135.3	312.9	301.3
$2As_4Se_3 = 2As_4 + {}^3/_4Se_8$	257.9	254.0	139.5	212.4	200.5

Table S5. Energy difference between $(HQ)_2EE(QH)_2$ and (HQ)(Q)HEEH(Q)(QH) isomers $\Delta E°_0$, (kJ mol^{-1}). B3LYP/def2-SVP level of theory.

E	Q	B3LYP/def2-SVP	B3LYP/def2-TZVPPD
P	O	-0.7	-50.0
P	S	47.1	19.0
P	Se	45.6	18.8
As	O	269.4	285.7
As	S	182.7	187.1
As	Se	164.3	151.9

Table S6. Planarization energies of one P or As center (ΔE, kJ mol^{-1}). B3LYP/def2-SVP level of theory.

Compound	ΔE
1	117.4
2	106.2
3	158.6
4	146.0

Table S7. Total energies $Eº_0$, sum of electronic and thermal enthalpies $Hº_{298}$ (Hartree) and standard entropies $Sº_{298}$ (cal mol^{-1}K^{-1}). B3LYP/def2-SVP (ECP on Zr) level of theory (B3LYP/def2-TZVPPD values in parenthesis).

Compound	Point group	$Eº_0$	$Hº_{298}$	$Sº_{298}$
CO	$C_{\infty v}$	-113.225014	-113.216597	47.209
P_4	T_d	-1365.087187	-1365.075594	66.904
As_4	T_d	-8942.661644	-8942.651479	78.259
S_8	D_{4d}	-3184.691874	-3184.668127	103.979
Se_8	D_{4d}	-19210.50315	-19210.48134	129.882
As_4S_3	C_{3v}	-10136.98917	-10136.9693	101.08
As_4Se_3	C_{3v}	-16146.64944	-16146.63036	110.296
P_4S_3	C_{3v}	-2559.412911	-2559.391543	88.837

P_4Se_3	C_{3v}	-8569.064169	-8569.043813	98.257
$[Cp''_2Zr(CO)_2]$	C_2	-1288.981257	-1288.313801	216.926
$[(Cp''_2Zr)_2(\mu,\eta^{1:1:1:1}\text{-}P_2S_4)]$ (**1**)	C_i	-4400.059761	-4398.743423	391.03
1_planar_P	C_1	-4400.015036		
$[(Cp''_2Zr)_2(\mu,\eta^{1:1:1:1}\text{-}P_2Se_4)]$ (**2**)	C_i	-12412.90224	-12411.58704	401.661
2_planar_P	C_1	-12412.8618037		
$[(Cp''_2Zr)_2(\mu,\eta^{1:1:1:1}\text{-}As_2S_4)]$ (**3**)	C_1	-8188.848478	-8187.533079	396.898
3_planar_As	C_1	-8188.788068		
$[(Cp''_2Zr)_2(\mu,\eta^{1:1:1:1}\text{-}As_2Se_4)]$ (**4**)	C_1	-16201.69783	-16200.38353	406.408
4_planar_As	C_1	-16201.64222		
$(HO)_2PP(OH)_2$	C_i	-985.6404176	-985.57149	91.893
	C_i	(-986.3017400)	(-986.23261)	(91.452)
(HO)(O)HPPH(O)(OH)	C_2	-985.6407028	-985.574076	82.196
	C_2	(-986.3207865)	(-986.253807)	(84.506)
$(HO)_2AsAs(OH)_2$	C_i	-4774.3832302	-4774.31689	102.183
	C_i	(-4775.3543726)	(-4775.287826)	(102.206)
(HO)(O)HAsAsH(O)(OH)	C_2	-4774.2806051	-4774.219161	89.957
	C_2	(-4775.2455423)	(-4775.184177)	(93.105)
$(HS)_2PP(SH)_2$	C_i	-2277.317767	-2277.264583	110.273
	C_i	(-2278.131443)	(-2278.078076)	(108.57)
(HS)(S)HPPH(S)(SH)	C_2	-2277.299818	-2277.245184	100.052
	C_2	(-2278.124209)	(-2278.069331)	(100.993)
$(HS)_2AsAs(SH)_2$	C_i	-6066.106273	-6066.054364	119.195
	C_i	(-6067.232632)	(-6067.180556)	(117.065)
(HS)(S)HAsAsH(S)(SH)	C_2	-6066.034967	-6065.984233	107.444
	C_2	(-6067.161383)	(-6067.11037)	(107.654)
$(HSe)_2PP(SeH)_2$	C_i	-10290.17063	-10290.12174	123.114
	C_i	(-10291.60048)	(-10291.551591)	(121.953)
(HSe)(Se)HPPH(Se)(SeH)	C_2	-10290.15127	-10290.09983	115.222
	C_2	(-10291.59334)	(-10291.541595)	(114.327)
$(HSe)_2AsAs(SeH)_2$	C_i	-14078.96634	-14078.91941	127.217
	C_i	(-14080.71159)	(-14080.66354)	(129.241)
(HSe)(Se)HAsAsH(Se)(SeH)	C_2	-14078.90486	-14078.8566	120.156
	C_2	(-14080.65372)	(-14080.60559)	(120.266)

Table S8. Optimized geometries of theoretically studied compounds. xyz coordinates in angstroms. B3LYP/def2-SVP (ECP on Zr) level of theory.

CO

6	0.000000000	0.000000000	-0.645940000
8	0.000000000	0.000000000	0.484455000

P_4

15	0.785647000	0.785647000	0.785647000
15	-0.785647000	-0.785647000	0.785647000
15	0.785647000	-0.785647000	-0.785647000
15	-0.785647000	0.785647000	-0.785647000

As_4

33	0.870395000	0.870395000	0.870395000
33	-0.870395000	-0.870395000	0.870395000
33	0.870395000	-0.870395000	-0.870395000
33	-0.870395000	0.870395000	-0.870395000

S_8

16	0.000000000	2.406257000	0.504416000
16	-1.701480000	1.701480000	-0.504416000
16	1.701480000	1.701480000	-0.504416000
16	-2.406257000	0.000000000	0.504416000
16	2.406257000	0.000000000	0.504416000
16	1.701480000	-1.701480000	-0.504416000
16	-1.701480000	-1.701480000	-0.504416000
16	0.000000000	-2.406257000	0.504416000

Se_8

34	0.000000000	2.695897000	0.579112000
34	-1.906287000	1.906287000	-0.579112000
34	1.906287000	1.906287000	-0.579112000
34	-2.695897000	0.000000000	0.579112000
34	2.695897000	0.000000000	0.579112000
34	1.906287000	-1.906287000	-0.579112000
34	-1.906287000	-1.906287000	-0.579112000
34	0.000000000	-2.695897000	0.579112000

As_4S_3

33	0.000000000	-0.000000000	2.097592000
16	0.000000000	1.989236000	0.998643000
16	1.722729000	-0.994618000	0.998643000
16	-1.722729000	-0.994618000	0.998643000
33	1.260535000	-0.727770000	-1.183388000
33	0.000000000	1.455541000	-1.183388000
33	-1.260535000	-0.727770000	-1.183388000

As_4Se_3

33	0.000000000	-0.000000000	1.956797000
34	0.000000000	2.110144000	0.805164000
34	1.827438000	-1.055072000	0.805164000
34	-1.827438000	-1.055072000	0.805164000
33	1.257545000	-0.726044000	-1.481829000
33	0.000000000	1.452088000	-1.481829000
33	-1.257545000	-0.726044000	-1.481829000

P_4S_3

15	0.000000000	0.000000000	1.735000000
16	-0.000000000	1.890489000	0.715004000
16	1.637212000	-0.945245000	0.715004000
16	-1.637212000	-0.945245000	0.715004000
15	1.142438000	-0.659587000	-1.341004000
15	0.000000000	1.319173000	-1.341004000
15	-1.142438000	-0.659587000	-1.341004000

P_4Se_3

15	0.000000000	-0.000000000	1.584150000
34	0.000000000	2.022339000	0.502667000
34	1.751397000	-1.011170000	0.502667000
34	-1.751397000	-1.011170000	0.502667000
15	1.139572000	-0.657932000	-1.667428000
15	0.000000000	1.315864000	-1.667428000
15	-1.139572000	-0.657932000	-1.667428000

$[Cp''_2Zr(CO)_2]$

40	0.000001000	0.000034000	0.031489000
1	1.234800000	-0.599420000	-2.781707000
6	1.628678000	-0.398078000	-1.785899000
6	1.967382000	-1.379811000	-0.803818000
1	1.872677000	1.826787000	-1.843086000
6	2.093184000	-2.887076000	-1.058142000
6	2.492163000	-0.645877000	0.312590000
1	2.887217000	-1.095223000	1.220795000
6	2.543781000	0.747940000	0.004073000
6	3.362207000	1.803921000	0.753799000
6	1.974397000	0.894670000	-1.290469000

6	-2.093272000	2.887077000	-1.058119000
6	-1.967424000	1.379815000	-0.803798000
6	-2.492165000	0.645859000	0.312618000
1	-1.234838000	0.599448000	-2.781698000
1	-2.887217000	1.095192000	1.220829000
6	-2.543745000	-0.747957000	0.004092000
6	-3.362116000	-1.803974000	0.753827000
6	-1.974378000	-0.894663000	-1.290459000
1	-1.872636000	-1.826776000	-1.843078000
6	-1.628705000	0.398095000	-1.785888000
6	3.473940000	1.493976000	2.259133000
6	2.802105000	3.225748000	0.556125000
6	4.788604000	1.756385000	0.144735000
6	0.824187000	-3.464007000	-1.714242000
6	2.380014000	-3.664141000	0.239419000
6	3.290402000	-3.089755000	-2.021220000
1	2.483871000	-4.738199000	0.016991000
1	1.571077000	-3.551583000	0.974437000
1	3.320198000	-3.336781000	0.709959000
1	3.450412000	-4.162351000	-2.221564000
1	4.217881000	-2.681771000	-1.589131000
1	3.119921000	-2.585877000	-2.985415000
1	0.971605000	-4.526840000	-1.966621000
1	0.569561000	-2.936931000	-2.647629000
1	-0.036266000	-3.388631000	-1.033265000
1	5.237899000	0.757834000	0.262028000
1	5.445100000	2.487529000	0.645064000
1	4.770134000	1.992891000	-0.930538000
1	3.945224000	0.515362000	2.438918000
1	2.496163000	1.497538000	2.759775000
1	4.103771000	2.252270000	2.751273000
1	1.796480000	3.336609000	0.984213000
1	2.752308000	3.497963000	-0.509598000
1	3.459734000	3.960069000	1.048373000
6	-3.290499000	3.089718000	-2.021192000
6	-0.824296000	3.464047000	-1.714229000
6	-2.380119000	3.664139000	0.239440000
6	-4.788578000	-1.756374000	0.144912000
6	-3.473682000	-1.494125000	2.259190000
6	-2.802064000	-3.225799000	0.556000000
1	-3.459672000	-3.960144000	1.048242000
1	-1.796406000	-3.336726000	0.983993000
1	-2.752365000	-3.497927000	-0.509750000
1	-4.103442000	-2.252461000	2.751355000
1	-3.944962000	-0.515530000	2.439088000
1	-2.495845000	-1.497699000	2.759720000
1	-5.445033000	-2.487540000	0.645260000
1	-4.770226000	-1.992806000	-0.930379000
1	-5.237844000	-0.757823000	0.262320000
1	-3.320281000	3.336740000	0.709998000
1	-2.484029000	4.738192000	0.017007000
1	-1.571164000	3.551626000	0.974445000
1	-0.569653000	2.936969000	-2.647611000
1	0.036164000	3.388715000	-1.033255000
1	-0.971756000	4.526871000	-1.966620000
1	-4.217966000	2.681714000	-1.589096000
1	-3.120009000	2.585837000	-2.985383000
1	-3.450537000	4.162309000	-2.221545000
6	-0.013593000	-1.455553000	1.669507000
6	0.013617000	1.455633000	1.669490000
8	0.032265000	-2.194707000	2.559016000
8	-0.032295000	2.194733000	2.559041000

$[(Cp''_2Zr)_2(\mu,\eta^{1:1:1:1}\text{-}P_2S_4)]$ (**1**)

40	-3.144833000	0.172261000	1.907956000

16	-0.699151000	0.390449000	2.522515000
16	-2.274359000	-1.273191000	0.024988000
15	-0.299749000	-0.808126000	0.769542000
6	-3.125022000	-1.655781000	3.825657000
1	-2.192026000	-2.101830000	4.161859000
6	-2.121745000	3.919799000	1.921560000
6	-4.356286000	1.529963000	-0.006106000
6	-3.103384000	2.187988000	0.186417000
1	-2.311741000	2.252846000	-0.555860000
6	-4.955957000	1.049846000	-1.332214000
6	-3.065898000	2.798601000	1.473017000
6	-3.971646000	-2.199032000	2.823028000
6	-3.723133000	-0.488560000	4.395517000
6	-4.923324000	-0.265440000	3.669461000
1	-5.647922000	0.522398000	3.860186000
6	-5.065639000	1.659869000	1.217211000
1	-6.074329000	1.300062000	1.413246000
6	-3.344133000	0.139596000	5.741620000
6	-4.274517000	2.423483000	2.126820000
1	-4.592374000	2.745810000	3.115994000
6	-0.758408000	3.861958000	1.211899000
1	-0.211226000	2.943352000	1.461819000
1	-0.142200000	4.721808000	1.520582000
1	-0.863811000	3.910913000	0.117445000
6	-2.822565000	5.246243000	1.524477000
1	-2.994486000	5.292695000	0.437788000
1	-2.195608000	6.108099000	1.807428000
1	-3.797741000	5.353481000	2.025291000
6	-1.900597000	3.924179000	3.444886000
1	-2.847178000	4.033430000	3.996806000
1	-1.260462000	4.774551000	3.729117000
1	-1.402920000	3.003625000	3.781978000
6	-5.691334000	-0.296119000	-1.177825000
1	-4.998130000	-1.105122000	-0.906581000
1	-6.178365000	-0.574600000	-2.126310000
1	-6.478915000	-0.244247000	-0.408788000
6	-3.914982000	-3.636369000	2.293849000
6	-1.821199000	0.220439000	5.950366000
1	-1.338158000	-0.763009000	5.851072000
1	-1.601812000	0.597054000	6.962520000
1	-1.343465000	0.894617000	5.226098000
6	-5.062780000	-1.287868000	2.687673000
1	-5.911393000	-1.398940000	2.014278000
6	-3.886378000	0.931003000	-2.432568000
1	-3.411797000	1.903312000	-2.637842000
1	-4.352271000	0.588369000	-3.370485000
1	-3.098261000	0.215806000	-2.158774000
6	-5.984428000	2.126148000	-1.765926000
1	-6.803151000	2.222990000	-1.035552000
1	-6.427115000	1.860921000	-2.740421000
1	-5.505022000	3.112539000	-1.867211000
6	-2.472628000	-4.172337000	2.218243000
1	-1.862432000	-3.582322000	1.520756000
1	-2.481388000	-5.217310000	1.868610000
1	-1.983242000	-4.164429000	3.204829000
6	-4.599508000	-3.792476000	0.923589000
1	-5.642133000	-3.437917000	0.944351000
1	-4.624076000	-4.856770000	0.639298000
1	-4.056699000	-3.247999000	0.139430000
6	-3.942502000	-0.786055000	6.833201000
1	-5.035267000	-0.873010000	6.726692000
1	-3.726507000	-0.384779000	7.837394000
1	-3.516446000	-1.799384000	6.772474000
6	-3.950108000	1.544111000	5.913910000
1	-3.546398000	2.251861000	5.176692000

1	-3.709573000	1.936252000	6.914761000
1	-5.047658000	1.535081000	5.823548000
6	-4.701228000	-4.490268000	3.324925000
1	-4.253258000	-4.418527000	4.328395000
1	-4.695958000	-5.551052000	3.023707000
1	-5.750206000	-4.162405000	3.399268000
16	0.699151000	-0.390449000	-2.522515000
16	2.274359000	1.273191000	-0.024988000
15	0.299749000	0.808126000	-0.769542000
40	3.144833000	-0.172261000	-1.907956000
6	3.125022000	1.655781000	-3.825657000
1	2.192026000	2.101830000	-4.161859000
6	2.121745000	-3.919799000	-1.921560000
6	4.356286000	-1.529963000	0.006106000
6	3.103384000	-2.187988000	-0.186417000
1	2.311741000	-2.252846000	0.555860000
6	4.955957000	-1.049846000	1.332214000
6	3.065898000	-2.798601000	-1.473017000
6	3.971646000	2.199032000	-2.823028000
6	3.723133000	0.488560000	-4.395517000
6	4.923324000	0.265440000	-3.669461000
1	5.647922000	-0.522398000	-3.860186000
6	5.065639000	-1.659869000	-1.217211000
1	6.074329000	-1.300062000	-1.413246000
6	3.344133000	-0.139596000	-5.741620000
6	4.274517000	-2.423483000	-2.126820000
1	4.592374000	-2.745810000	-3.115994000
6	0.758408000	-3.861958000	-1.211899000
1	0.211226000	-2.943352000	-1.461819000
1	0.142200000	-4.721808000	-1.520582000
1	0.863811000	-3.910913000	-0.117445000
6	2.822565000	-5.246243000	-1.524477000
1	2.994486000	-5.292695000	-0.437788000
1	2.195608000	-6.108099000	-1.807428000
1	3.797741000	-5.353481000	-2.025291000
6	1.900597000	-3.924179000	-3.444886000
1	2.847178000	-4.033430000	-3.996806000
1	1.260462000	-4.774551000	-3.729117000
1	1.402920000	-3.003625000	-3.781978000
6	5.691334000	0.296119000	1.177825000
1	4.998130000	1.105122000	0.906581000
1	6.178365000	0.574600000	2.126310000
1	6.478915000	0.244247000	0.408788000
6	3.914982000	3.636369000	-2.293849000
6	1.821199000	-0.220439000	-5.950366000
1	1.338158000	0.763009000	-5.851072000
1	1.601812000	-0.597054000	-6.962520000
1	1.343465000	-0.894617000	-5.226098000
6	5.062780000	1.287868000	-2.687673000
1	5.911393000	1.398940000	-2.014278000
6	3.886378000	-0.931003000	2.432568000
1	3.411797000	-1.903312000	2.637842000
1	4.352271000	-0.588369000	3.370485000
1	3.098261000	-0.215806000	2.158774000
6	5.984428000	-2.126148000	1.765926000
1	6.803151000	-2.222990000	1.035552000
1	6.427115000	-1.860921000	2.740421000
1	5.505022000	-3.112539000	1.867211000
6	2.472628000	4.172337000	-2.218243000
1	1.862432000	3.582322000	-1.520756000
1	2.481388000	5.217310000	-1.868610000
1	1.983242000	4.164429000	-3.204829000
6	4.599508000	3.792476000	-0.923589000
1	5.642133000	3.437917000	-0.944351000
1	4.624076000	4.856770000	-0.639298000

1	4.056699000	3.247999000	-0.139430000
6	3.942502000	0.786055000	-6.833201000
1	5.035267000	0.873010000	-6.726692000
1	3.726507000	0.384779000	-7.837394000
1	3.516446000	1.799384000	-6.772474000
6	3.950108000	-1.544111000	-5.913910000
1	3.546398000	-2.251861000	-5.176692000
1	3.709573000	-1.936252000	-6.914761000
1	5.047658000	-1.535081000	-5.823548000
6	4.701228000	4.490268000	-3.324925000
1	4.253258000	4.418527000	-4.328395000
1	4.695958000	5.551052000	-3.023707000
1	5.750206000	4.162405000	-3.399268000

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15	-0.950108000	0.026174000	-0.004583000
15	0.950235000	1.345701000	-0.124255000
16	-1.878012000	-0.771386000	-1.671694000
16	-1.874986000	-0.462769000	1.779206000
40	-3.582361000	0.412607000	-0.041101000
6	-5.882572000	-0.444898000	-0.706475000
6	-4.691494000	2.651337000	0.473934000
6	-3.341208000	2.876519000	0.870845000
6	-2.564241000	2.821002000	-0.326844000
6	-3.415579000	2.629111000	-1.457132000
6	-3.044865000	2.924243000	-2.914746000
6	-1.550039000	2.681005000	-3.191487000
6	-3.351572000	4.426040000	-3.150120000
6	-3.881228000	2.093821000	-3.902758000
6	-4.736616000	2.500028000	-0.936988000
1	-1.498311000	3.022846000	-0.382398000
6	-2.878483000	3.483697000	2.200318000
1	-0.908597000	3.318926000	-2.563347000
1	-1.318535000	2.923043000	-4.241459000
1	-1.274622000	1.631787000	-3.013986000
1	-5.643357000	2.372520000	-1.524431000
6	-5.919246000	-0.253002000	0.709373000
6	-5.158481000	-1.284742000	1.325131000
6	-4.607254000	-2.063351000	0.266255000
6	-5.236911000	-1.703532000	2.798443000
1	-3.956545000	-2.923022000	0.399773000
6	-5.103250000	-1.602325000	-0.985572000
1	-6.524617000	0.489772000	1.225180000
6	-5.121857000	-2.402555000	-2.293604000
6	-4.249604000	-2.841834000	3.118422000
6	-6.676408000	-2.233350000	3.027325000
6	-4.991630000	-0.531378000	3.763887000
6	-4.101237000	-3.556181000	-2.270685000
6	-6.540994000	-3.018740000	-2.406041000
6	-4.874307000	-1.524913000	-3.532657000
1	-6.453255000	0.127964000	-1.434848000
1	-3.076949000	-3.188844000	-2.115905000
1	-4.130952000	-4.101195000	-3.228035000
1	-4.331777000	-4.280431000	-1.473882000
1	-5.555778000	2.656048000	1.134463000
6	-1.386349000	3.221117000	2.474324000
1	-1.186080000	2.148854000	2.609805000
1	-1.076700000	3.745900000	3.392799000
1	-0.746748000	3.592470000	1.658614000
1	-6.771362000	-3.643687000	-1.528851000
1	-6.612659000	-3.652985000	-3.305552000
1	-7.315481000	-2.239198000	-2.476896000
1	-4.483138000	-3.751450000	2.543243000
1	-4.312695000	-3.103438000	4.187082000
1	-3.211747000	-2.554454000	2.896681000

6	-3.702372000	2.965719000	3.390087000
6	-3.095336000	5.014535000	2.077484000
1	-7.426959000	-1.443391000	2.868537000
1	-6.787627000	-2.605973000	4.059411000
1	-6.908022000	-3.060957000	2.338523000
1	-3.951228000	-0.182080000	3.709258000
1	-5.188832000	-0.845128000	4.802103000
1	-5.650655000	0.323468000	3.546500000
1	-4.417461000	4.648272000	-2.983576000
1	-3.100402000	4.713534000	-4.184986000
1	-2.765131000	5.062036000	-2.468375000
1	-3.672949000	1.021901000	-3.795023000
1	-3.643393000	2.383638000	-4.939134000
1	-4.962327000	2.252003000	-3.760075000
1	-4.779155000	3.161933000	3.264290000
1	-3.385797000	3.469042000	4.317993000
1	-3.561987000	1.885835000	3.525565000
1	-5.577663000	-0.679327000	-3.583595000
1	-5.005254000	-2.119281000	-4.451680000
1	-3.853455000	-1.117843000	-3.537682000
1	-2.505066000	5.433891000	1.247568000
1	-2.786565000	5.522979000	3.006346000
1	-4.154236000	5.254381000	1.891765000
16	2.058891000	0.517402000	-1.752430000
40	3.632955000	-0.410467000	0.025383000
16	2.039508000	0.779669000	1.622416000
6	6.003056000	0.013199000	0.795666000
6	4.325875000	-2.769356000	-0.516153000
6	2.973378000	-2.783120000	-0.957429000
6	2.170316000	-2.596314000	0.206611000
6	2.994387000	-2.606180000	1.371312000
6	2.528527000	-2.888539000	2.803257000
6	1.040464000	-2.555856000	3.000525000
6	2.722274000	-4.413649000	3.015880000
6	3.363458000	-2.137168000	3.852615000
6	4.337677000	-2.664989000	0.908723000
1	1.084320000	-2.536577000	0.211360000
6	2.485680000	-3.264589000	-2.328147000
1	0.397628000	-3.147812000	2.331798000
1	0.739514000	-2.791401000	4.033897000
1	0.828161000	-1.493977000	2.817208000
1	5.225975000	-2.734251000	1.533491000
6	6.049050000	-0.126427000	-0.625135000
6	5.485683000	1.042468000	-1.212942000
6	5.036584000	1.854111000	-0.132359000
6	5.659183000	1.501350000	-2.664468000
1	4.539183000	2.814038000	-0.242741000
6	5.412877000	1.270202000	1.109690000
1	6.539764000	-0.938308000	-1.158096000
6	5.498989000	2.004643000	2.452535000
6	4.784080000	2.727800000	-2.983049000
6	7.148388000	1.909582000	-2.811151000
6	5.355458000	0.383163000	-3.675151000
6	4.648562000	3.288452000	2.453479000
6	6.988436000	2.402226000	2.626776000
6	5.087907000	1.122049000	3.642996000
1	6.446971000	-0.678616000	1.508851000
1	3.588475000	3.068087000	2.263033000
1	4.724860000	3.784755000	3.434011000
1	4.998075000	4.007558000	1.696224000
1	5.203251000	-2.929766000	-1.139605000
6	0.979458000	-3.026887000	-2.518333000
1	0.721911000	-1.961066000	-2.455031000
1	0.665823000	-3.393072000	-3.509011000
1	0.381271000	-3.565188000	-1.767589000

1	7.340045000	3.011761000	1.779546000
1	7.118572000	2.992390000	3.548945000
1	7.637348000	1.515129000	2.696698000
1	5.058634000	3.594036000	-2.361048000
1	4.926064000	3.024086000	-4.034576000
1	3.717128000	2.512921000	-2.827752000
6	3.252761000	-2.618267000	-3.494317000
6	2.751054000	-4.793671000	-2.353399000
1	7.820155000	1.052841000	-2.645167000
1	7.337802000	2.299605000	-3.824872000
1	7.418109000	2.694912000	-2.087686000
1	4.290621000	0.116526000	-3.665968000
1	5.608974000	0.714163000	-4.695067000
1	5.940369000	-0.527651000	-3.471342000
1	3.782784000	-4.702328000	2.942657000
1	2.357081000	-4.706104000	4.014161000
1	2.161394000	-4.993095000	2.266014000
1	3.210078000	-1.053135000	3.778507000
1	3.065462000	-2.449015000	4.866457000
1	4.441208000	-2.342230000	3.750490000
1	4.344194000	-2.695231000	-3.369270000
1	2.993903000	-3.121189000	-4.439823000
1	2.990137000	-1.556882000	-3.599758000
1	5.636089000	0.167357000	3.658729000
1	5.303872000	1.641010000	4.590680000
1	4.011932000	0.902693000	3.621253000
1	2.236284000	-5.299798000	-1.521641000
1	2.380097000	-5.226675000	-3.296983000
1	3.825885000	-5.020872000	-2.273936000

[(Cp″$_2$Zr)$_2$(μ,η$^{1:1:1:1}$-P$_2$Se$_4$)] (**2**)

40	1.699734000	1.266419000	-3.160771000
34	-0.206920000	2.240051000	-1.565317000
34	0.825190000	-1.145345000	-2.403606000
15	-0.573081000	0.036292000	-0.997158000
6	4.609339000	-0.762827000	-1.449017000
6	0.129266000	2.340038000	-5.066858000
6	0.063745000	0.933129000	-5.262211000
1	-0.840204000	0.334828000	-5.185143000
6	3.979245000	0.547003000	-1.937757000
6	3.383034000	1.548933000	-1.119646000
1	3.046661000	1.397712000	-0.096800000
6	3.376606000	2.801454000	-1.807755000
6	3.950572000	-1.291200000	-0.164341000
1	4.002329000	-0.559380000	0.655989000
1	4.471872000	-2.201323000	0.173148000
1	2.895559000	-1.546091000	-0.330401000
6	4.227109000	1.159941000	-3.199326000
1	4.712048000	0.687977000	-4.051863000
6	1.499393000	2.700531000	-5.231028000
1	1.903635000	3.710630000	-5.188359000
6	1.338577000	0.432993000	-5.662613000
6	-1.067612000	3.297622000	-5.099402000
6	1.609588000	-0.912520000	-6.343791000
6	2.231857000	1.538032000	-5.613562000
1	3.281463000	1.526448000	-5.900454000
6	0.463809000	-1.912358000	-6.103378000
1	0.299987000	-2.093997000	-5.031182000
1	0.698860000	-2.874979000	-6.585133000
1	-0.482972000	-1.552369000	-6.535189000
6	3.876537000	2.540596000	-3.110992000
1	4.043789000	3.279390000	-3.892439000
6	2.543619000	4.118994000	0.203673000
1	1.545455000	3.661250000	0.153373000
1	2.437875000	5.133294000	0.620875000

1	3.151299000	3.534790000	0.912175000
6	1.697883000	-0.627124000	-7.865476000
1	0.774980000	-0.152382000	-8.233921000
1	1.843291000	-1.567602000	-8.422541000
1	2.539269000	0.042557000	-8.103007000
6	-2.361078000	2.623751000	-4.604599000
1	-2.636888000	1.763633000	-5.234731000
1	-3.196568000	3.340759000	-4.650493000
1	-2.260054000	2.277958000	-3.566429000
6	3.208798000	4.190880000	-1.182548000
6	-1.256426000	3.675428000	-6.593574000
1	-0.372150000	4.198118000	-6.991016000
1	-2.127922000	4.340822000	-6.710726000
1	-1.425709000	2.780241000	-7.212208000
6	-0.821694000	4.594094000	-4.307282000
1	-0.752725000	4.401298000	-3.228090000
1	-1.657310000	5.294237000	-4.467252000
1	0.098514000	5.105289000	-4.630317000
6	6.089171000	-0.415952000	-1.132398000
1	6.623249000	-0.068411000	-2.030809000
1	6.613431000	-1.305741000	-0.746021000
1	6.156471000	0.376930000	-0.371129000
6	4.588819000	-1.870026000	-2.516289000
1	3.560128000	-2.189273000	-2.733738000
1	5.143424000	-2.750020000	-2.153034000
1	5.063262000	-1.549749000	-3.456677000
6	2.408716000	5.143386000	-2.090808000
1	2.860605000	5.229920000	-3.092021000
1	2.384866000	6.154945000	-1.654375000
1	1.370035000	4.806965000	-2.212840000
6	2.937622000	-1.537839000	-5.883817000
1	3.785728000	-0.849208000	-6.025809000
1	3.153906000	-2.448499000	-6.465560000
1	2.901191000	-1.819244000	-4.823085000
6	4.638505000	4.766153000	-1.007258000
1	5.258676000	4.102678000	-0.384373000
1	4.595423000	5.752507000	-0.516140000
1	5.146523000	4.890733000	-1.976478000
34	0.206920000	-2.240051000	1.565317000
34	-0.825190000	1.145345000	2.403606000
15	0.573081000	-0.036292000	0.997158000
40	-1.699734000	-1.266419000	3.160771000
6	-4.609339000	0.762827000	1.449017000
6	-0.129266000	-2.340038000	5.066858000
6	-0.063745000	-0.933129000	5.262211000
1	0.840204000	-0.334828000	5.185143000
6	-3.979245000	-0.547003000	1.937757000
6	-3.383034000	-1.548933000	1.119646000
1	-3.046661000	-1.397712000	0.096800000
6	-3.376606000	-2.801454000	1.807755000
6	-3.950572000	1.291200000	0.164341000
1	-4.002329000	0.559380000	-0.655989000
1	-4.471872000	2.201323000	-0.173148000
1	-2.895559000	1.546091000	0.330401000
6	-4.227109000	-1.159941000	3.199326000
1	-4.712048000	-0.687977000	4.051863000
6	-1.499393000	-2.700531000	5.231028000
1	-1.903635000	-3.710630000	5.188359000
6	-1.338577000	-0.432993000	5.662613000
6	1.067612000	-3.297622000	5.099402000
6	-1.609588000	0.912520000	6.343791000
6	-2.231857000	-1.538032000	5.613562000
1	-3.281463000	-1.526448000	5.900454000
6	-0.463809000	1.912358000	6.103378000
1	-0.299987000	2.093997000	5.031182000

1	-0.698860000	2.874979000	6.585133000
1	0.482972000	1.552369000	6.535189000
6	-3.876537000	-2.540596000	3.110992000
1	-4.043789000	-3.279390000	3.892439000
6	-2.543619000	-4.118994000	-0.203673000
1	-1.545455000	-3.661250000	-0.153373000
1	-2.437875000	-5.133294000	-0.620875000
1	-3.151299000	-3.534790000	-0.912175000
6	-1.697883000	0.627124000	7.865476000
1	-0.774980000	0.152382000	8.233921000
1	-1.843291000	1.567602000	8.422541000
1	-2.539269000	-0.042557000	8.103007000
6	2.361078000	-2.623751000	4.604599000
1	2.636888000	-1.763633000	5.234731000
1	3.196568000	-3.340759000	4.650493000
1	2.260054000	-2.277958000	3.566429000
6	-3.208798000	-4.190880000	1.182548000
6	1.256426000	-3.675428000	6.593574000
1	0.372150000	-4.198118000	6.991016000
1	2.127922000	-4.340822000	6.710726000
1	1.425709000	-2.780241000	7.212208000
6	0.821694000	-4.594094000	4.307282000
1	0.752725000	-4.401298000	3.228090000
1	1.657310000	-5.294237000	4.467252000
1	-0.098514000	-5.105289000	4.630317000
6	-6.089171000	0.415952000	1.132398000
1	-6.623249000	0.068411000	2.030809000
1	-6.613431000	1.305741000	0.746021000
1	-6.156471000	-0.376930000	0.371129000
6	-4.588819000	1.870026000	2.516289000
1	-3.560128000	2.189273000	2.733738000
1	-5.143424000	2.750020000	2.153034000
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1	-1.370035000	-4.806965000	2.212840000
6	-2.937622000	1.537839000	5.883817000
1	-3.785728000	0.849208000	6.025809000
1	-3.153906000	2.448499000	6.465560000
1	-2.901191000	1.819244000	4.823085000
6	-4.638505000	-4.766153000	1.007258000
1	-5.258676000	-4.102678000	0.384373000
1	-4.595423000	-5.752507000	0.516140000
1	-5.146523000	-4.890733000	1.976478000

2_planar_P

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34	-1.964200000	-1.771722000	0.851524000
40	-3.713115000	0.291149000	0.296552000
6	-6.050891000	0.297254000	-0.692250000
6	-4.829412000	1.347849000	2.314858000
6	-3.501898000	1.139094000	2.790868000
6	-2.672232000	2.021315000	2.034202000
6	-3.466143000	2.810414000	1.149743000
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6	-3.501384000	5.253973000	1.496327000
6	-3.726068000	4.383169000	-0.843803000
6	-4.806397000	2.354768000	1.314855000
1	-1.606092000	2.155227000	2.192092000
6	-3.124156000	0.494200000	4.129940000
1	-0.997946000	4.183156000	1.311388000

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1	-5.681198000	2.767040000	0.817256000
6	-6.042723000	-0.719000000	0.309419000
6	-5.295209000	-1.829336000	-0.172988000
6	-4.789204000	-1.446551000	-1.448883000
6	-5.388692000	-3.261455000	0.369317000
1	-4.163075000	-2.067952000	-2.083156000
6	-5.301841000	-0.168262000	-1.813890000
1	-6.611582000	-0.690437000	1.236565000
6	-5.388315000	0.387819000	-3.240493000
6	-4.415238000	-4.213791000	-0.351723000
6	-6.833196000	-3.741763000	0.068602000
6	-5.160406000	-3.340778000	1.888199000
6	-4.390981000	-0.306510000	-4.186799000
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6	-5.182871000	1.911383000	-3.304435000
1	-6.628113000	1.217963000	-0.644855000
1	-3.352723000	-0.193363000	-3.843090000
1	-4.468561000	0.128364000	-5.196328000
1	-4.604141000	-1.383005000	-4.277363000
1	-5.726940000	0.874796000	2.706198000
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1	-1.438492000	-0.745544000	3.472412000
1	-1.384766000	-0.273066000	5.190512000
1	-0.969929000	0.909321000	3.937513000
1	-7.026321000	-1.012721000	-3.692865000
1	-6.946632000	0.395042000	-4.785411000
1	-7.584667000	0.580777000	-3.130907000
1	-4.657501000	-4.299787000	-1.422573000
1	-4.488582000	-5.223702000	0.083028000
1	-3.371549000	-3.879436000	-0.266083000
6	-4.006427000	-0.721430000	4.461609000
6	-3.355847000	1.581417000	5.211096000
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1	-5.371821000	-4.359576000	2.251789000
1	-5.820498000	-2.650772000	2.435953000
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1	-5.074320000	-0.454541000	4.512735000
1	-3.727869000	-1.134088000	5.444729000
1	-3.886054000	-1.516658000	3.714581000
1	-5.848538000	2.444323000	-2.608127000
1	-5.402402000	2.281152000	-4.319281000
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1	-4.406541000	1.911338000	5.227963000
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6	2.230909000	-1.793883000	-1.894976000
6	3.037892000	-2.735305000	-1.187242000
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1	1.146316000	-1.736249000	-1.841117000
6	2.574143000	-0.287956000	-4.037073000
1	0.460643000	-3.884460000	-1.144883000
1	0.736698000	-4.924727000	0.266214000
1	0.778769000	-3.155081000	0.447138000
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6	6.142427000	0.407684000	-0.624878000
6	5.610492000	1.586168000	-0.029712000
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6	5.783718000	3.016508000	-0.556754000
1	4.776657000	1.901844000	2.015011000
6	5.631311000	-0.111802000	1.572814000
1	6.576716000	0.334300000	-1.619635000
6	5.826157000	-0.721158000	2.966442000
6	4.988827000	4.033188000	0.283050000
6	7.294315000	3.342230000	-0.418543000
6	5.393945000	3.159486000	-2.037833000
6	5.000377000	0.016029000	4.037226000
6	7.329890000	-0.545250000	3.304186000
6	5.491752000	-2.222447000	3.005674000
1	6.603486000	-1.612379000	0.217143000
1	3.922774000	-0.038639000	3.825605000
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1	5.284901000	1.077305000	4.109417000
1	5.274309000	-1.025476000	-3.021597000
6	1.071183000	0.030754000	-3.990865000
1	0.809012000	0.639789000	-3.115873000
1	0.777894000	0.589011000	-4.894310000
1	0.460893000	-0.884644000	-3.959853000
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1	7.542911000	-0.947125000	4.308522000
1	7.970228000	-1.075228000	2.581973000
1	5.338172000	4.057288000	1.327053000
1	5.123405000	5.045627000	-0.129920000
1	3.913748000	3.802598000	0.281859000
6	3.365532000	1.002768000	-4.310953000
6	2.827157000	-1.270460000	-5.211946000
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1	7.627648000	3.246312000	0.626619000
1	4.312692000	3.037386000	-2.184935000
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6	4.684805000	2.244219000	-0.524302000
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1	3.577470000	-5.940734000	1.953125000
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1	5.335031000	-0.952462000	-4.916675000
1	6.241392000	-0.755542000	-3.404781000
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1	6.337047000	1.071124000	-1.488845000
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1	-6.124184000	-4.822716000	2.516694000
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3_planar_As

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6	4.141806000	-2.108186000	1.959739000
6	3.109958000	-2.616545000	1.113163000
6	3.634126000	-2.908901000	-0.184109000
6	2.995934000	-3.826813000	-1.234032000
6	1.459354000	-3.735185000	-1.249880000
6	3.394479000	-5.274108000	-0.843753000
6	3.522601000	-3.539895000	-2.652089000
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6	4.589693000	2.055981000	-0.977419000
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6	5.939255000	4.323349000	1.062750000
6	4.629822000	3.042626000	2.769445000
6	4.317282000	1.126595000	-3.951131000
6	6.673710000	1.849820000	-3.505803000
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1	3.549205000	0.349701000	-3.825767000
1	4.584984000	1.164397000	-5.019761000
1	3.862816000	2.093861000	-3.689870000
1	6.299127000	-1.712870000	1.476714000
6	2.654985000	-1.955121000	4.014222000
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1	2.659408000	-1.860945000	5.112228000
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1	6.327664000	2.882799000	-3.345657000
1	6.933860000	1.740360000	-4.571954000
1	7.586342000	1.701657000	-2.907850000
1	3.532355000	4.555486000	-0.174798000
1	3.308871000	5.042315000	1.514117000
1	2.551870000	3.537802000	0.917861000
6	4.886789000	-0.809353000	4.022214000

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1	-5.011709000	-4.681961000	-1.947726000
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6	-2.241449000	2.360541000	-0.831225000
6	-3.032542000	2.924722000	0.214239000
6	-2.508514000	3.727069000	1.411265000
6	-1.039541000	3.401554000	1.726851000
6	-2.593945000	5.215509000	0.976164000

6	-3.360588000	3.543585000	2.678666000
6	-4.372409000	2.934868000	-0.260649000
1	-1.169071000	2.182427000	-0.776161000
6	-2.542029000	2.040037000	-3.436512000
1	-0.377318000	3.633327000	0.879349000
1	-0.699400000	4.006137000	2.582649000
1	-0.899261000	2.342679000	1.982424000
1	-5.231362000	3.345799000	0.265532000
6	-6.355477000	0.154628000	-0.821590000
6	-5.931586000	-1.204558000	-0.808869000
6	-5.608112000	-1.506347000	0.544985000
6	-6.165358000	-2.224322000	-1.929445000
1	-5.235579000	-2.465106000	0.895881000
6	-5.940983000	-0.404969000	1.385424000
1	-6.724718000	0.699123000	-1.688004000
6	-6.187453000	-0.476472000	2.897232000
6	-5.440218000	-3.555580000	-1.658022000
6	-7.692398000	-2.499979000	-1.941029000
6	-5.757236000	-1.687457000	-3.311893000
6	-5.482250000	-1.685568000	3.539433000
6	-7.718722000	-0.660506000	3.068846000
6	-5.768402000	0.810760000	3.627507000
1	-6.743295000	1.613626000	0.830013000
1	-4.394732000	-1.651723000	3.382836000
1	-5.672590000	-1.694828000	4.624415000
1	-5.860612000	-2.637084000	3.134335000
1	-5.247997000	2.471195000	-2.270303000
6	-1.069255000	1.602603000	-3.497123000
1	-0.914330000	0.617241000	-3.037283000
1	-0.740716000	1.543024000	-4.546978000
1	-0.407966000	2.319502000	-2.987947000
1	-8.073608000	-1.556555000	2.536013000
1	-7.969860000	-0.776563000	4.136116000
1	-8.276018000	0.206308000	2.680556000
1	-5.778102000	-4.015157000	-0.716177000
1	-5.660210000	-4.271159000	-2.466164000
1	-4.350464000	-3.421700000	-1.604850000
6	-3.397837000	1.090004000	-4.292033000
6	-2.650693000	3.467882000	-4.036842000
1	-8.266632000	-1.586563000	-2.161268000
1	-7.937048000	-3.250477000	-2.710722000
1	-8.033393000	-2.886846000	-0.967937000
1	-4.677789000	-1.493443000	-3.366824000
1	-6.003860000	-2.425101000	-4.092129000
1	-6.285979000	-0.754480000	-3.563934000
1	-3.637140000	5.535230000	0.824830000
1	-2.148231000	5.861267000	1.750587000
1	-2.047468000	5.386402000	0.035619000
1	-3.219520000	2.544659000	3.113402000
1	-3.064185000	4.282099000	3.440661000
1	-4.434847000	3.687110000	2.482783000
1	-4.470389000	1.335883000	-4.240245000
1	-3.095281000	1.160552000	-5.349085000
1	-3.267971000	0.045061000	-3.979921000
1	-6.229638000	1.705862000	3.181470000
1	-6.085926000	0.768218000	4.681692000
1	-4.678317000	0.944989000	3.614252000
1	-2.080265000	4.194444000	-3.437396000
1	-2.244105000	3.478807000	-5.061436000
1	-3.696019000	3.812114000	-4.081603000

$(HO)_2PP(OH)_2$

1	-1.140288000	-0.730873000	-2.517225000
8	-1.201706000	-0.670119000	-1.554255000
15	0.333523000	-0.587564000	-0.892383000

8	0.450048000	-2.026621000	-0.045126000
15	-0.333523000	0.587564000	0.892383000
8	-0.450048000	2.026621000	0.045126000
8	1.201706000	0.670119000	1.554255000
1	1.128048000	-2.587504000	-0.445895000
1	-1.128048000	2.587504000	0.445895000
1	1.140288000	0.730873000	2.517225000

(HO)(O)HPPH(O)(OH)

8	1.346267000	1.316523000	-0.493584000
8	-1.346267000	1.457130000	-0.255038000
8	1.346267000	-1.457130000	-0.255038000
8	-1.346267000	-1.316523000	-0.493584000
1	-1.706378000	0.638597000	-0.676458000
1	1.706378000	-0.638597000	-0.676458000
15	-0.112865000	-1.114067000	0.339531000
15	0.112865000	1.114067000	0.339531000
1	-0.077378000	-1.809126000	1.572470000
1	0.077378000	1.809126000	1.572470000

$(HO)_2AsAs(OH)_2$

1	-1.209288000	-0.846779000	-2.634157000
8	-1.263189000	-0.712953000	-1.677188000
33	0.414023000	-0.594134000	-0.995725000
8	0.495736000	-2.159581000	-0.082730000
33	-0.414023000	0.594134000	0.995725000
8	-0.495736000	2.159581000	0.082730000
8	1.263189000	0.712953000	1.677188000
1	1.113930000	-2.755799000	-0.528779000
1	-1.113930000	2.755799000	0.528779000
1	1.209288000	0.846779000	2.634157000

(HO)(O)HAsAsH(O)(OH)

8	-1.462364000	-1.366714000	-0.666473000
8	1.462364000	-1.486957000	-0.477254000
8	-1.462364000	1.486957000	-0.477254000
8	1.462364000	1.366714000	-0.666473000
1	1.753393000	-0.610211000	-0.833834000
1	-1.753393000	0.610211000	-0.833834000
33	0.112842000	1.225955000	0.258145000
33	-0.112842000	-1.225955000	0.258145000
1	0.015987000	2.139654000	1.464872000
1	-0.015987000	-2.139654000	1.464872000

$(HS)_2PP(SH)_2$

1	-1.342750000	-0.435051000	-2.996998000
16	-1.736667000	-0.624408000	-1.715636000
15	0.273373000	-0.595184000	-0.931108000
16	0.341491000	-2.565359000	-0.023688000
15	-0.273373000	0.595184000	0.931108000
16	-0.341491000	2.565359000	0.023688000
16	1.736667000	0.624408000	1.715636000
1	1.695365000	-2.612954000	-0.034693000
1	-1.695365000	2.612954000	0.034693000
1	1.342750000	0.435051000	2.996998000

(HS)(S)HPPH(S)(SH)

16	2.054858000	-0.804996000	0.972884000
16	-0.703625000	-2.504586000	-0.503823000
16	0.703625000	2.504586000	-0.503823000
16	-2.054858000	0.804996000	0.972884000
1	-1.359860000	-2.035464000	0.591408000
1	1.359860000	2.035464000	0.591408000
15	-0.703625000	0.904477000	-0.421358000
15	0.703625000	-0.904477000	-0.421358000
1	-1.143363000	0.960947000	-1.776010000
1	1.143363000	-0.960947000	-1.776010000

$(HS)_2AsAs(SH)_2$

1	-1.502893000	-0.418728000	-3.092772000
16	-1.838193000	-0.652091000	-1.801928000
33	0.322612000	-0.563453000	-1.070539000
16	0.395601000	-2.694723000	-0.210192000
33	-0.322612000	0.563453000	1.070539000
16	-0.395601000	2.694723000	0.210192000
16	1.838193000	0.652091000	1.801928000
1	1.683025000	-2.557919000	0.193107000
1	-1.683025000	2.557919000	-0.193107000
1	1.502893000	0.418728000	3.092772000

(HS)(S)HAsAsH(S)(SH)

16	0.571388000	-2.557485000	0.604605000
16	-2.602342000	-0.556430000	0.313651000
16	2.602342000	0.556430000	0.313651000
16	-0.571388000	2.557485000	0.604605000
1	-2.121211000	0.662532000	0.743494000
1	2.121211000	-0.662532000	0.743494000
33	0.571388000	1.152356000	-0.411023000
33	-0.571388000	-1.152356000	-0.411023000
1	0.836007000	1.486660000	-1.871822000
1	-0.836007000	-1.486660000	-1.871822000

$(HSe)_2PP(SeH)_2$

1	-1.469633000	-0.285949000	-3.126348000
34	-1.891230000	-0.657206000	-1.760343000
15	0.274154000	-0.552769000	-0.958546000
34	0.376112000	-2.705486000	-0.091971000
15	-0.274154000	0.552769000	0.958546000
34	-0.376112000	2.705486000	0.091971000
34	1.891230000	0.657206000	1.760343000
1	1.819865000	-2.587592000	0.207573000
1	-1.819865000	2.587592000	-0.207573000
1	1.469633000	0.285949000	3.126348000

(HSe)(Se)HPPH(Se)(SeH)

34	1.623013000	-1.584428000	1.098545000
34	-1.623013000	-2.217637000	-0.843387000
34	1.623013000	2.217637000	-0.843387000
34	-1.623013000	1.584428000	1.098545000
1	-2.125660000	-1.765066000	0.471270000
1	2.125660000	1.765066000	0.471270000
15	-0.350253000	1.094772000	-0.488797000
15	0.350253000	-1.094772000	-0.488797000
1	-0.862992000	1.205737000	-1.814708000
1	0.862992000	-1.205737000	-1.814708000

$(HSe)_2AsAs(SeH)_2$

1	-1.603271000	-0.254690000	-3.208876000
34	-1.970426000	-0.720062000	-1.855489000
33	0.319808000	-0.554080000	-1.078230000
34	0.429429000	-2.820579000	-0.193318000
33	-0.319808000	0.554080000	1.078230000
34	-0.429429000	2.820579000	0.193318000
34	1.970426000	0.720062000	1.855489000
1	1.782334000	-2.590441000	0.358943000
1	-1.782334000	2.590441000	-0.358943000
1	1.603271000	0.254690000	3.208876000

(HSe)(Se)HAsAsH(Se)(SeH)

34	0.635165000	2.892792000	0.254623000
34	-2.429190000	0.606828000	-0.884894000
34	2.429190000	-0.606828000	-0.884894000
34	-0.635165000	-2.892792000	0.254623000
1	-2.221372000	-0.855568000	-0.628185000
1	2.221372000	0.855568000	-0.628185000

33	0.635165000	-1.109950000	0.608027000
33	-0.635165000	1.109950000	0.608027000
1	1.270457000	-1.059869000	1.992512000
1	-1.270457000	1.059869000	1.992512000

6. IR spectra of compounds 1, 2 and 3

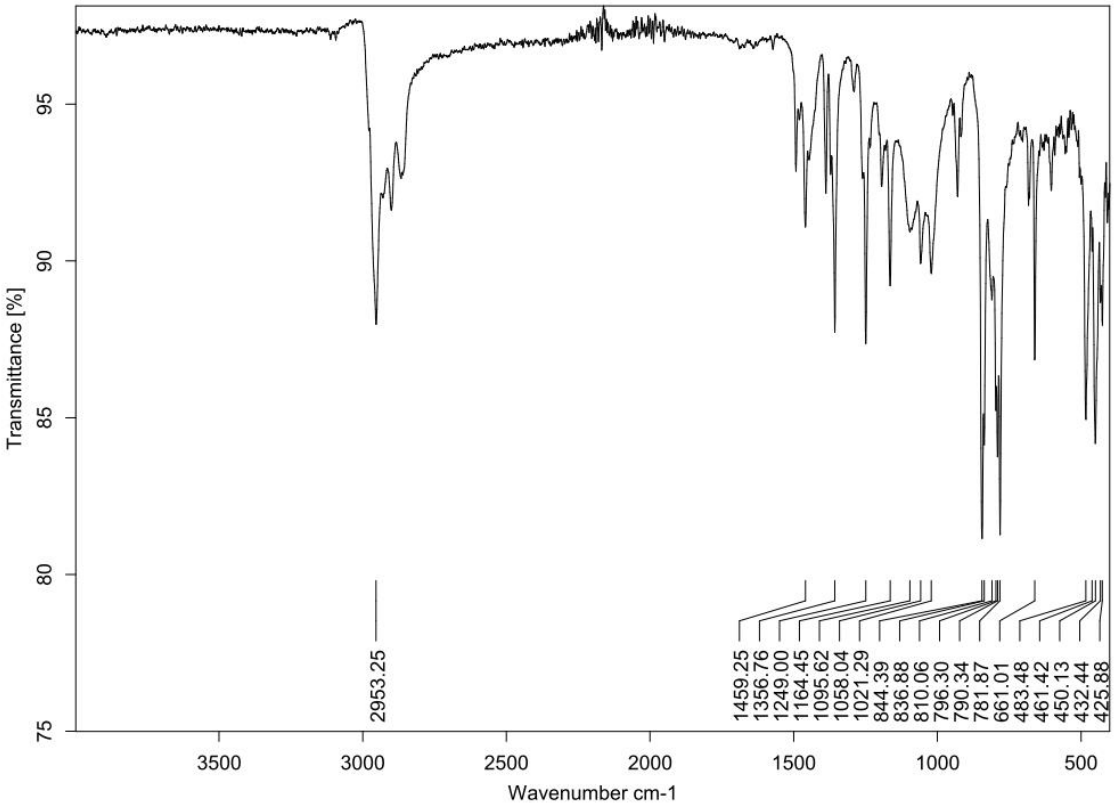

Fig. S17 IR spectrum of **1**.

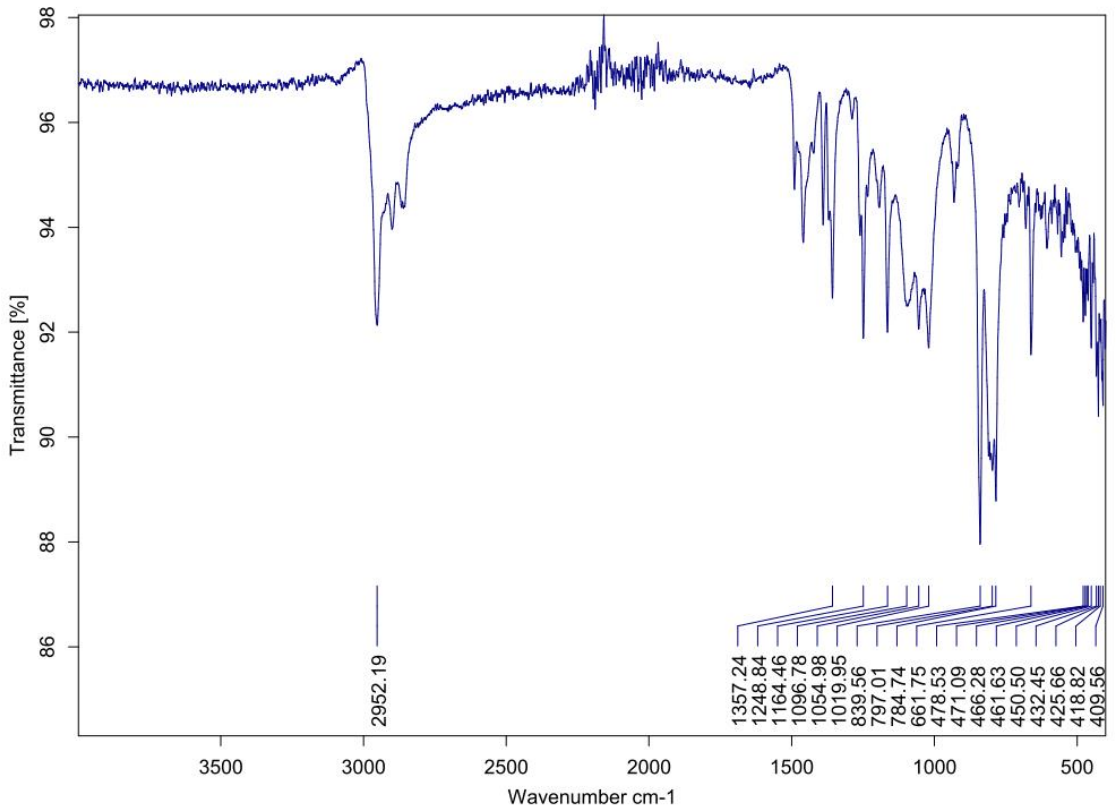

Fig. S18 IR spectrum of **2**.

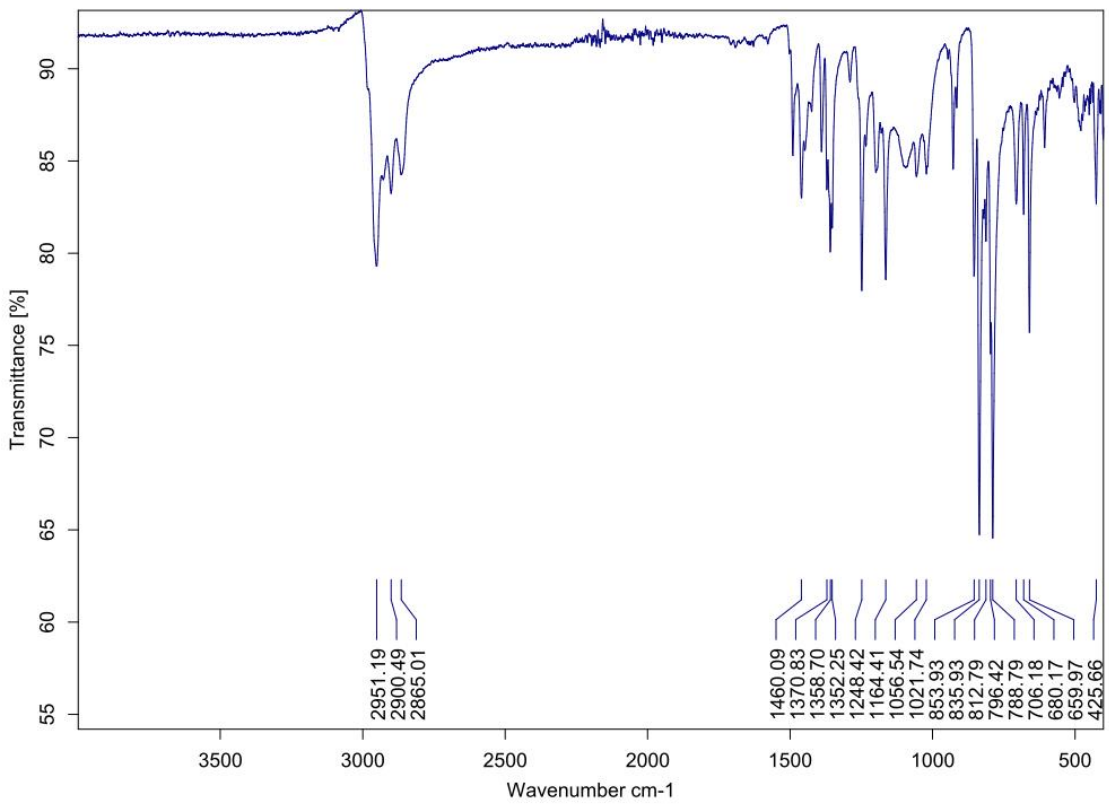

Fig. S19 IR spectrum of **3**.

7. References

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