Supporting Information for the paper entitled:

Reactivity of the Pentelidene Complexes [Cp*E{W(CO)$_5$}$_2$] (E = P, As) towards Dichalcogenides and Chalcogenols - Synthesis of Novel Chalcogenopentelidene Complexes

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1. General Information

1.1. Working techniques

The following reactions were carried out under an atmosphere of dry Nitrogen or Argon using standard Schlenk techniques. Traces of O_2 were eliminated by leading the inert gas (N_2 or Ar) through a copper catalyst heated to 145 °C, subsequently washing it with concentrated sulphuric acid and drying it with orange gel and phosphorus pentoxide.

Solvents were either collected from a solvent purification system (MBraun SPS 800) or dried, degassed and distilled according to standard techniques.

Before use, the diatomaceous earth required for filtration was stored at 110 °C. The silica gel 60 required for column chromatography (particle size 0.063-0.2 mm) was dried at 150 °C in vacuo for 3 d prior to use.

For photolytical reactions, a mercury vapor lamp from the Hanau company (type TQ 150) was used.

1.2. Methods of analysis

The NMR spectra were recorded on a BRUKER Avance 300 (^{1}H: 300.13 MHz, ^{13}C: 75.48 MHz, ^{31}P: 121.49 MHz) or Avance 400 (^{1}H: 400.13 MHz, ^{13}C: 100.61 MHz, ^{31}P: 161.98 MHz) spectrometer at room temperature unless stated otherwise. Chemical shifts δ refer to external standards of tetramethylsilane (^{1}H, ^{13}C NMR) and 85 % phosphoric acid (^{31}P NMR, ^{31}P{^{1}H} NMR), respectively, and are given in ppm. Coupling constants J are given in Hz without consideration of absolute signs. Analysis, Simulations and graphic representations of the spectra were prepared with *TopSpin 3.0*[1].

Infrared spectra were recorded in solution (CH_2Cl_2) with a ThermoScientific Nicolet iS5 spectrometer using the iD5 Transmission element or an ATR element equipped with a Ge crystal.

Mass spectra were recorded on a Jeol AccuTOF GCX (FD) spectrometer by the mass spectrometry department of the University of Regensburg or a ThermoQuest Finnigan MAT 95 spectrometer.

Elemental analysis was conducted by the microanalytics laboratory of the University of Regensburg with the Elementar Vario MICRO cube.

1.3. Starting Materials

The following substances were bought or synthesized according to standard techniques:

[Cp*P{W(CO)$_5$}$_2$] (**1a**)[2], [Cp*As{W(CO)$_5$}$_2$] (**1b**)[2], Ph_2S_2, PhSH, Ph_2Se_2, Mes_2Se_2[3], PhSeH, Mes_2Te_2[1], $Tipp_2Te_2$[4].

2. Experimental Data with NMR details

2.1 Synthesis of 2a

A solution of Ph_2S_2 (44 mg, 0.2 mmol) in 20 mL of toluene was added dropwise to a solution of **1a** (163 mg, 0.2 mmol) in 30 mL of toluene at room temperature. The mixture was stirred for two days, whereupon the blue solution turned violet. The solvent was removed in vacuo and the residue recrystallised from hexane at -28 °C, to give green, shiny crystals of [PhSP{W(CO)$_5$}$_2$] (**2a**). NMR yield: 21 mg (13 %)

Photolytical reaction: A mixture of **1a** (163 mg, 0.2 mmol) and Ph_2S_2 (44 mg, 0.2 mmol) in 50 mL of toluene was irradiated for 2 h with a TQ 150 Hg lamp until the reaction solution turned violet. The solution was then concentrated and stored at -28 °C, where a dark green powder of [PhSP{W(CO)$_5$}$_2$] (**2a**) could be obtained. NMR yield: 19 mg (12 %)

Chalkogenol reaction: A solution of PhSH (22 mg, 0.02 mL, 0.2 mmol) in 20 mL of toluene was added dropwise to a solution of **1a** (163 mg, 0.2 mmol) at -80 °C. The mixture was stirred and warmed to room temperature, whereupon the blue solution turned violet. After extraction of the dried reaction mixture with hexane, a few crystals of **2a** could be obtained by storing the concentrated hexane solution at -28 °C. NMR yield: 30 mg (19 %)

2a: ^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 7.55 (m, 3H), 7.65 (m, 2H); **^{31}P{^{1}H} NMR** (CD_2Cl_2, 162 MHz): δ = 822.9 (s, $^1J_{P,W}$ = 192 Hz); **^{31}P NMR** (CD_2Cl_2, 162 MHz): δ = 822.9 (s, $^1J_{P,W}$ = 192 Hz); **IR** (KBr) ν_{max}/cm^{-1} = 2962 w (CH), 2922 w (CH), 2852 w (CH), 2093 m (CO), 2055 s (CO), 1956 sh (CO), 1937 vs br (CO); **MS** (EI, 70eV): m/z (%): 787.7 (11) [M$^+$], 703.8 (9) [M$^+$-3CO], 678.7 (19) [P{W(CO)$_5$}$_2$$^+$], 650.7 (17) [P{W(CO)$_5$}$_2$$^+$-CO], 619.9 (29) [M$^+$-6CO], 591.8 (37) [M$^+$-7CO], 563.9 (29) [M$^+$-8CO], 535.9 (28) [M$^+$-9CO], 507.9 (60) [M$^+$-10CO], 481.9 (22) [P{W(CO)$_5$}$_2$$^+$-7CO], 352.0 (14) [W(CO)$_6$$^+$], 295.9 (12) [W(CO)$_6$$^+$-2CO], 268.0 (23) [W(CO)$_6$$^+$-3CO], 240.0 (9) [W(CO)$_6$$^+$-4CO], 212.0 (8) [W(CO)$_6$$^+$-5CO], 186.0 (12) [W(CO)$_6$$^+$-6CO], 110.0 (33) [PhSH$^+$], 78.1 (100) [Ph$^+$]; **elemental analysis** calcd (%) for $C_{16}H_5O_{10}PSW_2$ + 0.1 C_5H_{12}: C 24.98, H 0.80, S 4.03; found: C 25.43, H 0.68, S 3.99.

[1] Mes_2Te_2 was synthesized analogously to Mes_2Se_2.

^{1}H NMR spectrum of **2a**:

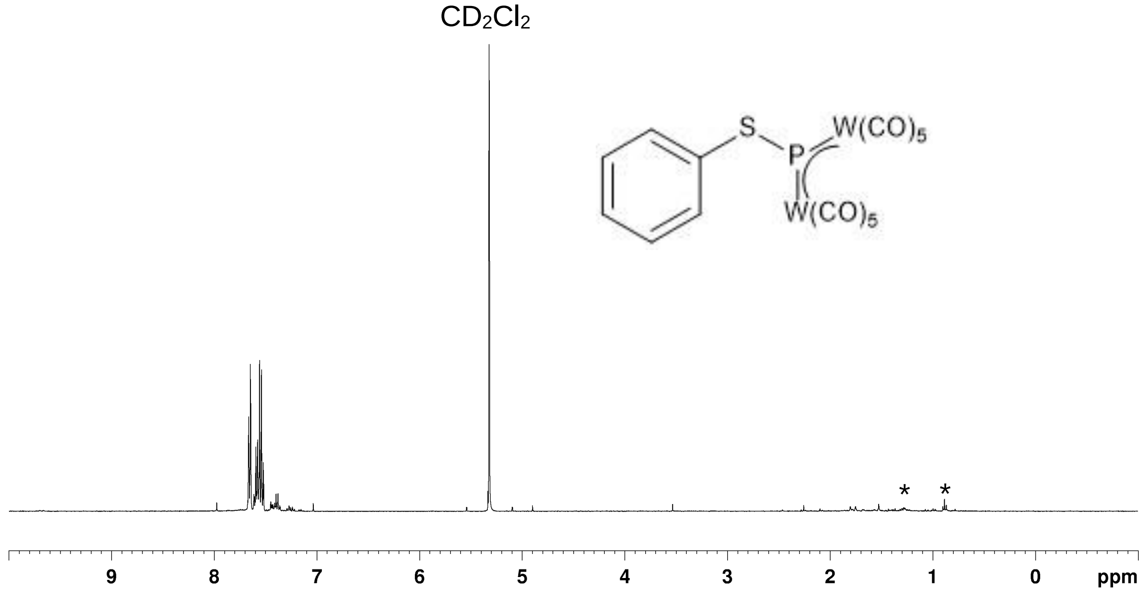


Figure S1. ^{1}H NMR spectrum of **2a** in CD_2Cl_2. * = pentane

$^{31}P\{^{1}H\}$ NMR spectrum of **2a**:

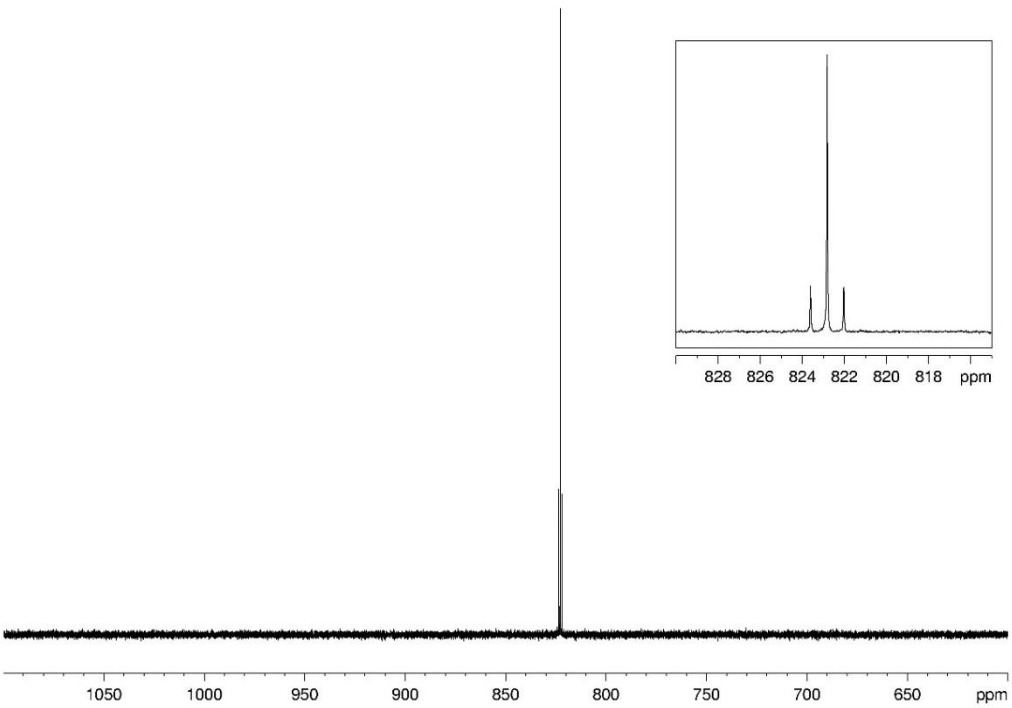


Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum of **2a** in CD_2Cl_2.

$^{31}P\{^1H\}$ NMR spectra of the reaction solutions:

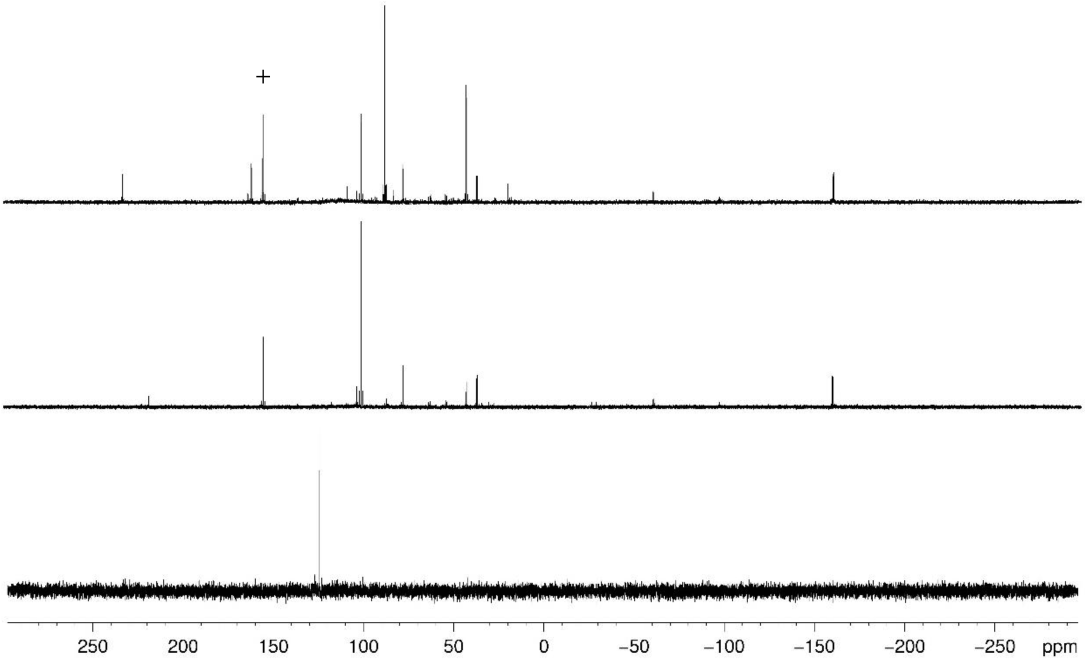


Figure S3. Section of the $^{31}P\{^1H\}$ NMR spectra of the reaction mixtures of **1a** + Ph_2S_2 in CD_2Cl_2. Bottom to top: Irradiation, stirring at room temp., heating to 90 °C. + = impurity in **1a**. Rest of the products could not be identified.

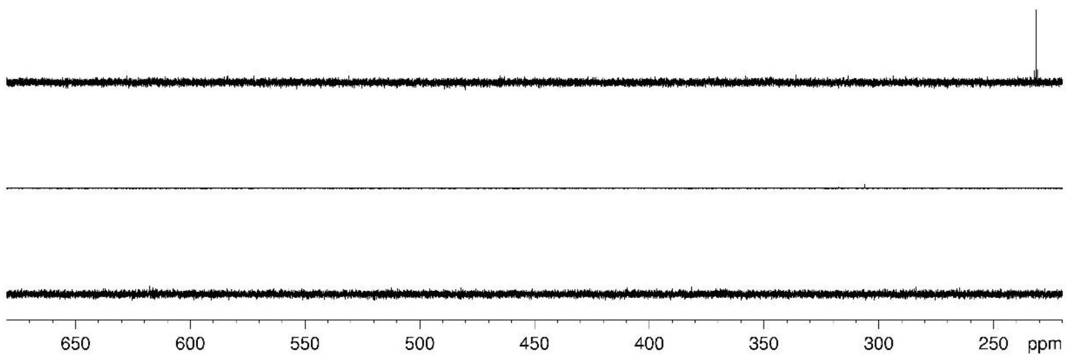


Figure S4. Section of the $^{31}P\{^1H\}$ NMR spectra of the reaction mixtures of **1a** with Ph_2S_2 in CD_2Cl_2. Bottom to top: Irradiation, stirring at room temp., heating to 90 °C.

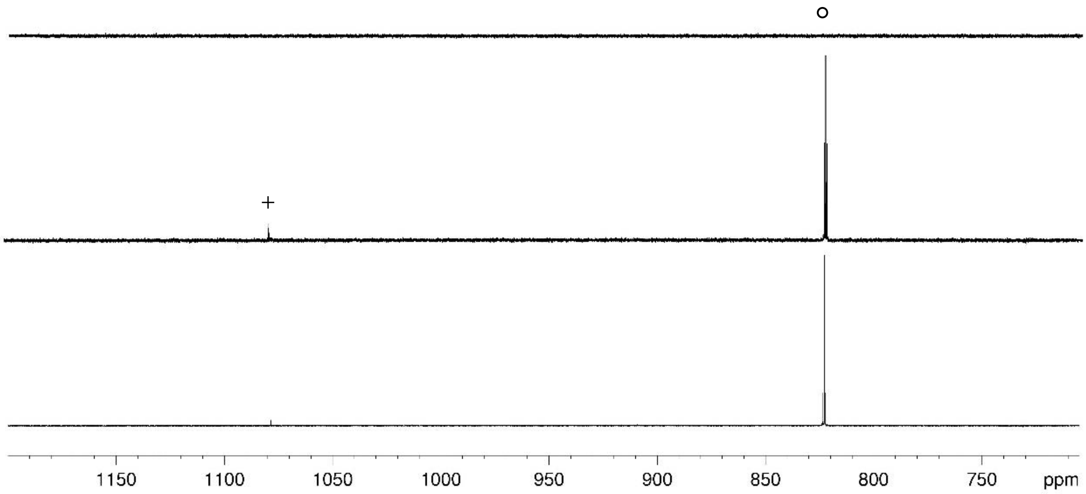


Figure S5. Part of the $^{31}P\{^1H\}$ NMR spectra of the reaction mixtures of **1a** + Ph_2S_2 in CD_2Cl_2. Bottom to top: Irradiation, stirring at room temp., heating to 90 °C. + = **1a**, ° = **2a**.

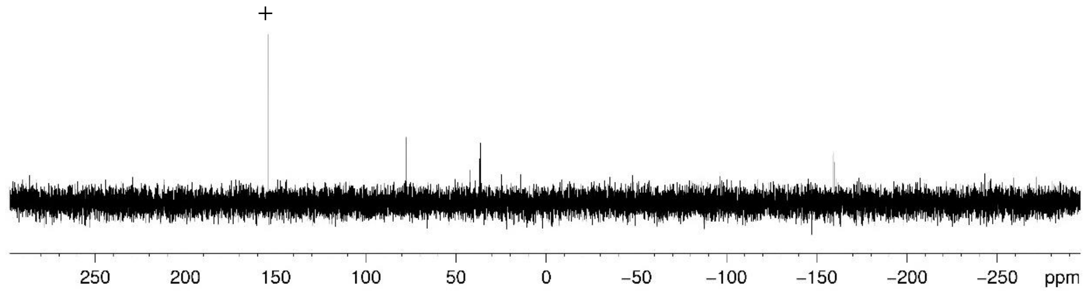


Figure S6. Part of the $^{31}P\{^1H\}$ NMR spectrum of the reaction mixture of **1a** + PhSH in in CD_2Cl_2. + = impurity in **1a**.

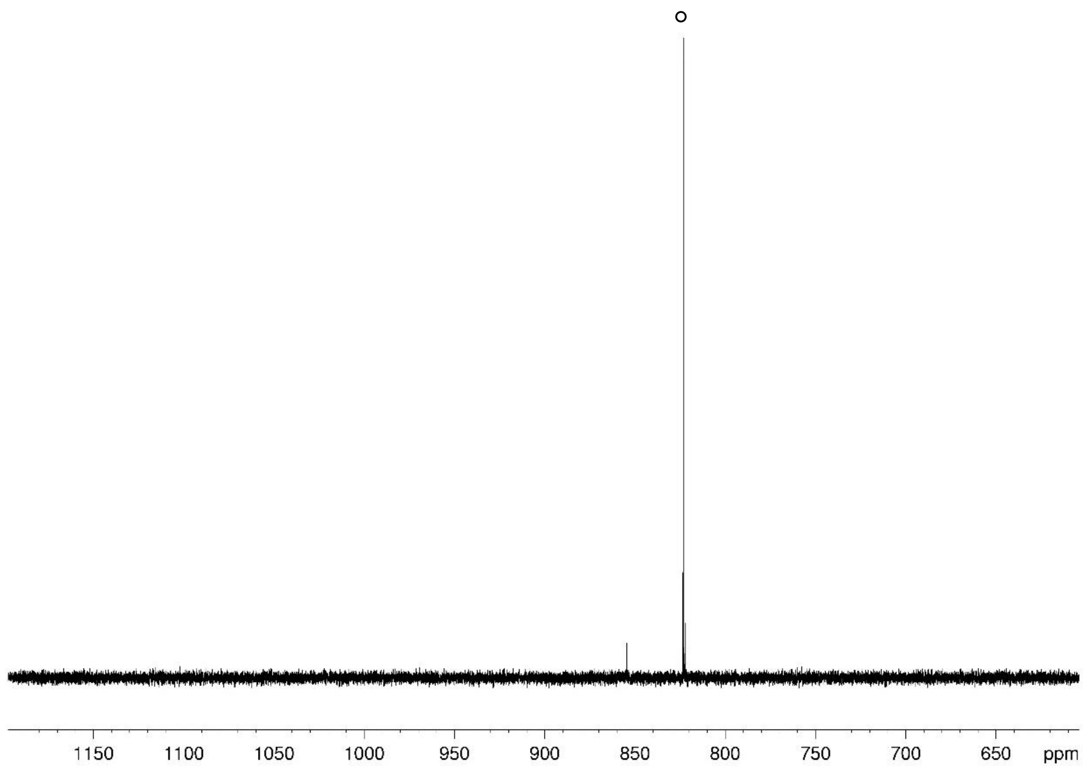


Figure S7. Part of the $^{31}P\{^{1}H\}$ NMR spectrum of the reaction mixture of **1a** + PhSH in CD_2Cl_2. ° = **2a**.

2.2 Reaction of 1b with Ph_2S_2

A solution of Ph_2S_2 (44 mg, 0.2 mmol) in 20 mL of toluene was added dropwise to a solution of **1b** (172 mg, 0.2 mmol) in 30 mL of toluene at room temperature. The mixture was stirred for two days, whereupon the blue solution turned violet. The solvent was removed in vacuo and the residue was dissolved again in hexane. After storing the solution at -28 °C, green shiny crystals of **2b** could be obtained. **Yield**: 17 mg (10 %).

Heating the reaction solution to 90 °C for 2h results in a brownish green solution. After removing the solvent and extracting the residue with hexane, the known compounds $[PhS\{W(CO)_4\}]_2$ (green blocks) and $(PhS)_3As$ (brown plates) were obtained as a few crystals each at – 28 °C from the hexane phase. Since there is no suitable NMR active nucleus present in the desired compound $[PhSAs\{W(CO)_5\}_2]$ (**2b**), we cannot say whether **2b** is formed or not in this reaction.

Chalkogenol reaction: A solution of PhSH (0.02 mL, 22 mg, 0.2 mmol) in 5 mL of toluene was added dropwise to a solution of **1b** (172 mg, 0.2 mmol) in 20 mL of toluene at – 80 °C. The solution was then warmed to -10 °C, where the blue solution turned violet. The solvent was removed in vacuo and the residue was extracted with hexane. Storing the violet hexane solution at -28 °C gave a few green shiny crystals of **2b**.

2b: ^{1}H NMR (C_6D_6, 400 MHz): δ = 7.01 (m, 3H), 7.19 (m, 2H); **IR** (KBr) ν_{max}/cm^{-1} = 2965 w (CH), 2918 w (CH), 2851 w (CH), 2091 m (CO), 2058 s (CO), 2017 sh (CO), 1970 sh (CO), 1933 vs (CO); **MS** (EI, 70eV): m/z (%): 831.5 (1) [M^+], 803.6 (1) [M^+-CO], 775.6 (1) [M^+-2CO], 722.6 (1) [M^+-PhS], 694.6 (1) [M^+-PhS-CO], 666.6 (1) [M^+-PhS-2CO], 635.7 (1) [M^+-7CO], 607.8 (1) [M^+-8CO], 579.7 (1) [M^+-9CO], 551.8 (1) [M^+-10CO], 442.8 (1) [M^+-PhS-10CO], 351.9 (1) [$W(CO)_6^+$], 295.9 (1) [$W(CO)_6^+$-2CO], 268.0 (2) [$W(CO)_6^+$-3CO], 239.9 (1) [$W(CO)_6^+$-4CO], 212.0 (1) [$W(CO)_6^+$-5CO]; **elemental analysis** calcd. (%) for $C_{16}H_5AsO_{10}SW_2$: C 23.10, H 0.61, S 3.85; found: C 23.33, H 0.70, S 3.82.

^{1}H NMR spectrum:

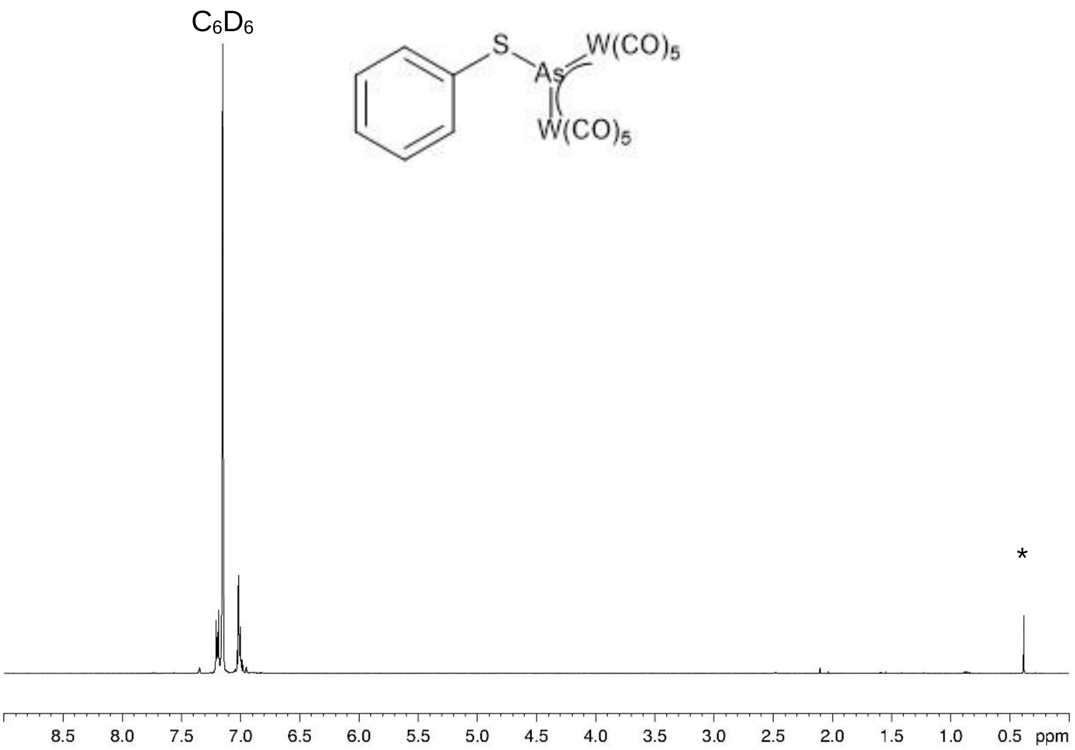


Figure S8. ^{1}H NMR spectrum of **2b** in C_6D_6. * = grease

2.3 Synthesis of 3a-I

A solution of PhSeH (0,02 mL, 31 mg, 0.2 mmol) in 20 mL of toluene was added dropwise to a solution of **1a** (163 mg, 0.2 mmol) in 30 mL of toluene at -80 °C. The mixture was stirred until the cooling bath reached –30 °C and the solution turned violet. After analyzing the reaction solution spectroscopically, it was stored at -28 °C and a few dark red plates of [PhSeP{W(CO)$_5$}$_2$] (**3a-I**) could be obtained. The rest of the solution was then spectroscopically characterized.

3a-I: Yield: 27 mg (15 %); **^{31}P{^{1}H} NMR** (C_6D_6, 162 MHz): δ = 835.0 (s, $^{1}J_{P,W}$ = 186 Hz, $^{1}J_{P,Se}$ = 488 Hz); **^{31}P NMR** (C_6D_6, 162 MHz): δ = 835.0 (s, $^{1}J_{P,W}$ = 186 Hz, $^{1}J_{P,Se}$ = 488 Hz).

^{1}H NMR spectrum of the reaction solution:

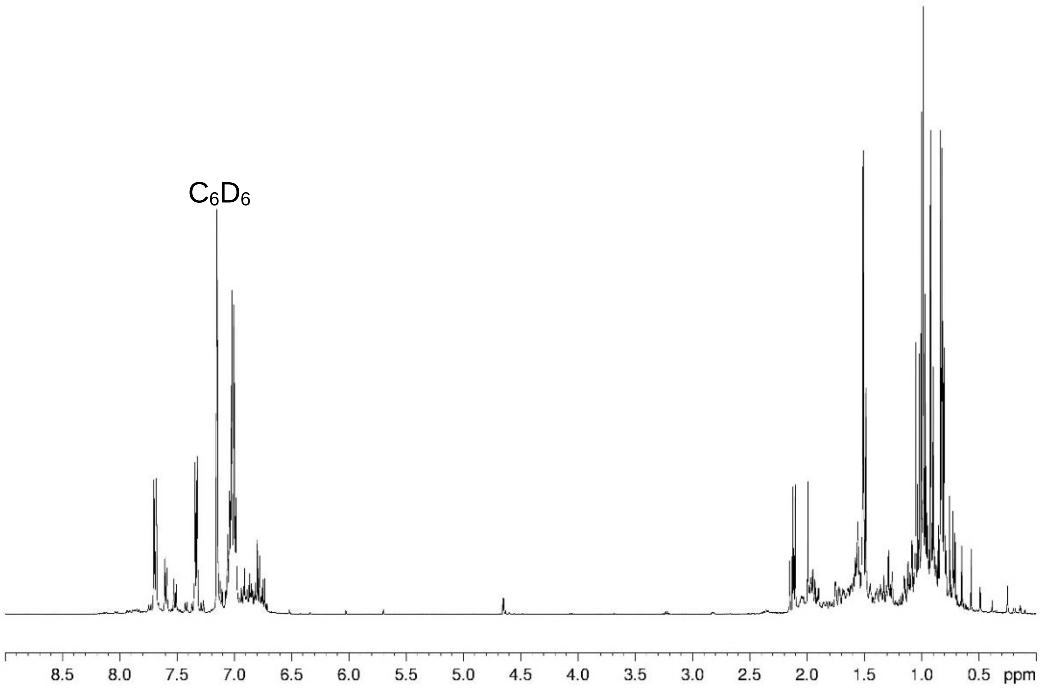


Figure S9. ^{1}H NMR spectrum of the reaction mixture of **1a** + PhSeH in C_6D_6

^{31}P{^{1}H} NMR spectrum of **3a-I**:

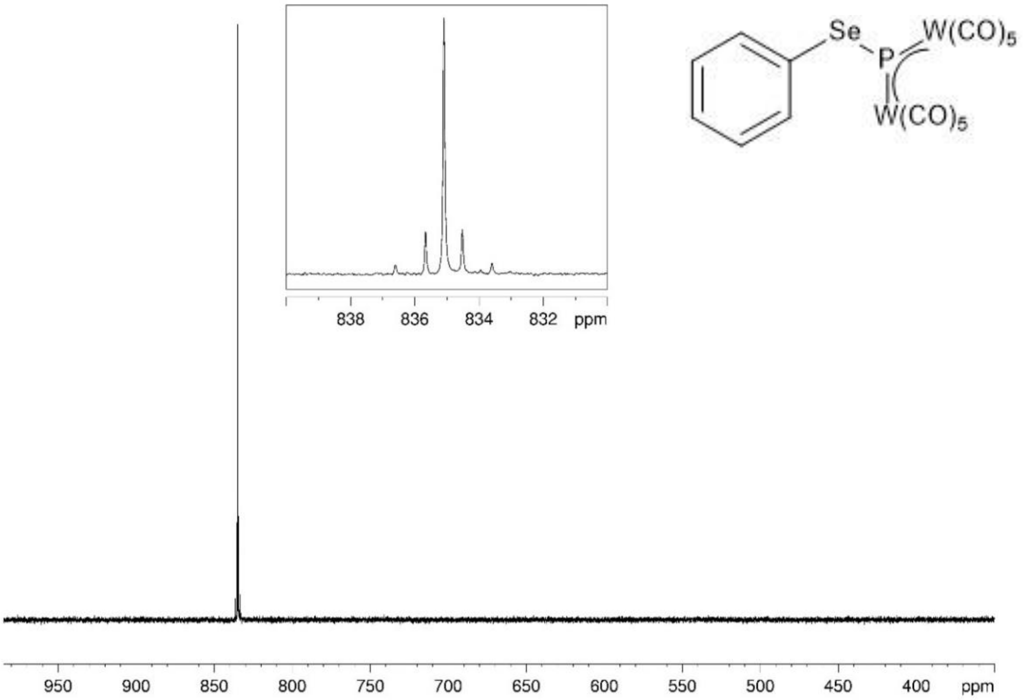
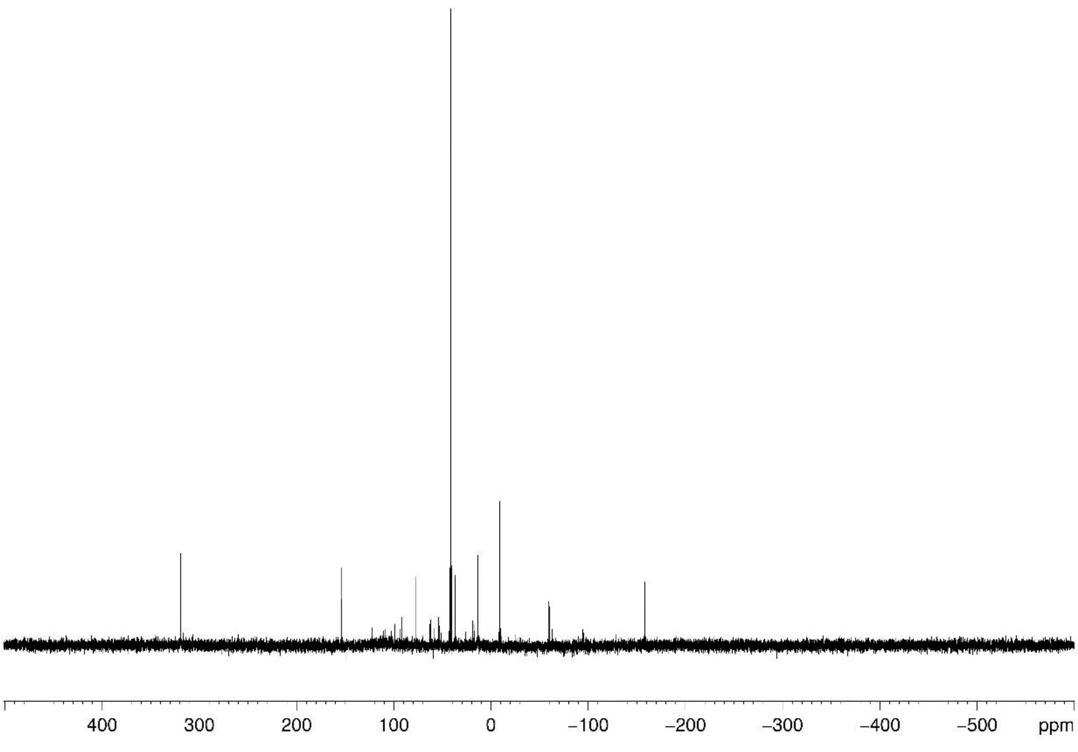


Figure S10. $^{31}P\{^1H\}$ NMR spectrum of **3a-I** in CD_2Cl_2.

<u>$^{31}P\{^1H\}$ NMR spectra of the reaction solution:</u>



o

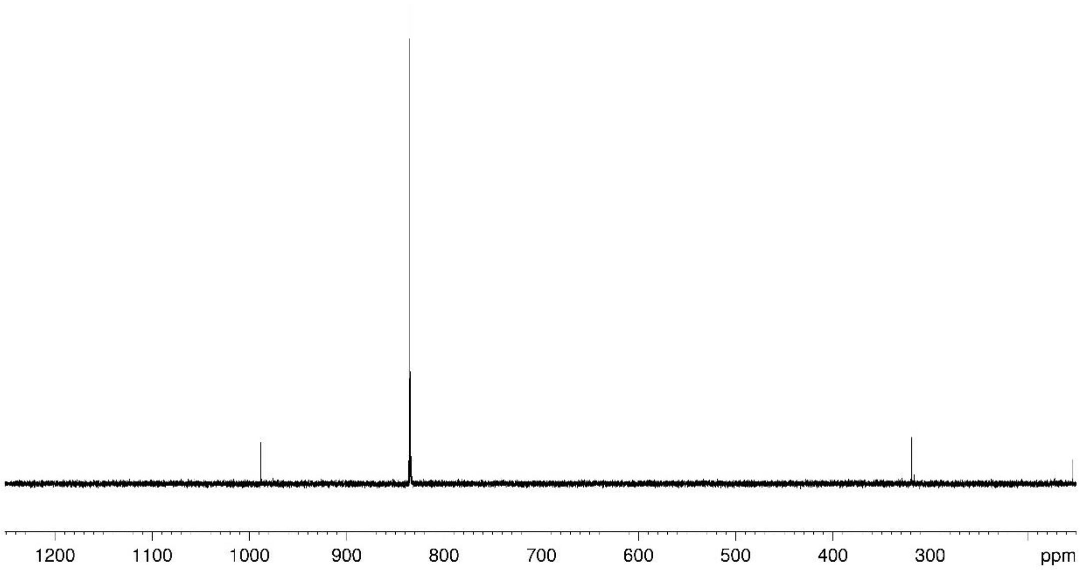


Figure S11. $^{31}P\{^{1}H\}$ NMR spectra of the reaction mixture of **1a** + PhSeH in CD_2Cl_2. ° = **3a-I**.

2.4 Synthesis of 3a-II

A solution of Mes_2Se_2 (160 mg, 0.4 mmol) in 20 mL of toluene was added dropwise to a solution of **1a** (326 mg, 0.4 mmol) in 30 mL of toluene at room temperature. The mixture was stirred for two days, whereupon the blue solution turned violet. After removing the solvent and recrystallizing from CH_2Cl_2 at -28 °C, green, shiny crystals of [MesSeP{W(CO)$_5$}$_2$] (**3a-II**) could be obtained.

3a-II: Yield: 57 mg (15%); **^{1}H NMR** (CD_2Cl_2, 400 MHz): δ = 2.32 (s, 3H, *p*-CH_3), 2.44 (s, 6H, *o*-CH_3), 7.10 (s, 2H, Mes); **^{31}P{^{1}H} NMR** (CD_2Cl_2, 162 MHz): δ = 854.3 (s, $^1J_{P,W}$ = 184 Hz, $^1J_{P,Se}$ = 507 Hz); **^{31}P NMR** (CD_2Cl_2, 162 MHz): δ = 854.3 (s, $^1J_{P,W}$ = 184 Hz, $^1J_{P,Se}$ = 507 Hz); **IR** (KBr) ν_{max}/cm^{-1} = 2957 w (CH), 2919 w (CH), 2850 w (CH), 2090 m (CO), 2053 s (CO), 2015 sh (CO), 1956 vs (CO), 1936 vs (CO); **MS** (EI, 70eV): m/z (%): 877.8 (2) [M$^+$], 678.9 (16) [P{W(CO)$_5$}$_2^+$], 651.0 (15) [P{W(CO)$_5$}$_2^+$-CO], 622.9 (8) [P{W(CO)$_5$}$_2^+$-2CO], 595.9 (17) [P{W(CO)$_5$}$_2^+$-3CO], 567.0 (4) [P{W(CO)$_5$}$_2^+$-4CO], 538.9 (3) [P{W(CO)$_5$}$_2^+$-5CO]; **elemental analysis** calcd. (%) for $C_{19}H_{11}O_{10}PSeW_2$: C 26.02, H 1.26; found: C 24.63, H 1.28.

<u>^{1}H NMR spectrum:</u>

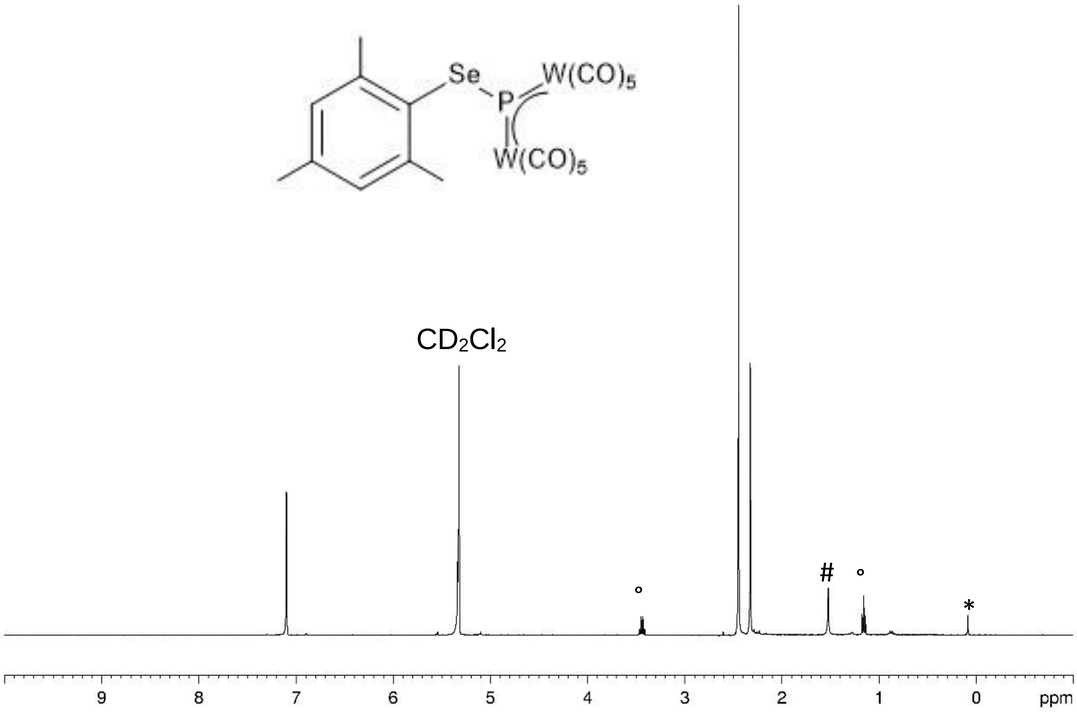


Figure S12. ^{1}H NMR spectrum of **3a-II** in CD_2Cl_2. ° = Et_2O, # = H_2O, * = grease

$^{31}P\{^1H\}$ NMR spectrum:

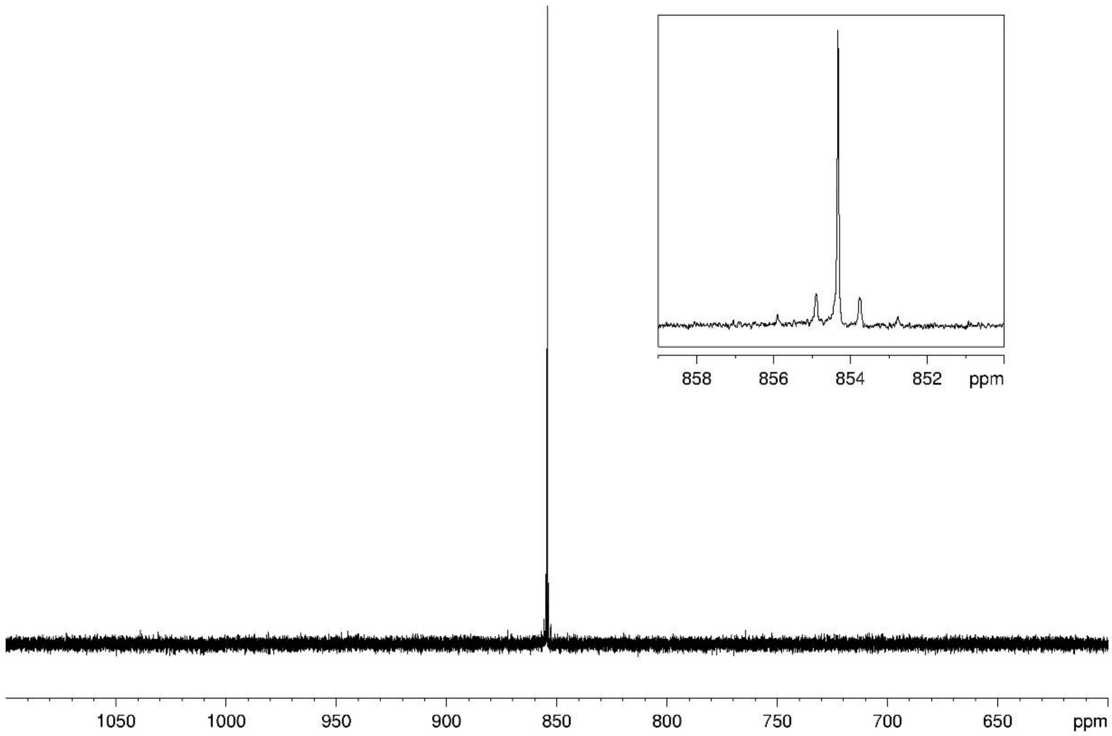


Figure S13. $^{31}P\{^1H\}$ NMR spectrum of **3a-II** in CD_2Cl_2.

2.5 Synthesis of 3b

A solution of Mes_2Se_2 (80 mg, 0.2 mmol) in 20 mL of toluene was added dropwise to a solution of **1b** (172 mg, 0.2 mmol) in 30 mL of toluene at room temperature. The mixture was stirred for two days, whereupon the blue solution turned violet. After recrystallizing from CH_2Cl_2 at -28 °C, green, shiny crystals of [MesSeAs{W(CO)$_5$}$_2$] (**3b**) could be obtained.

3b: Yield: 20 mg (11%); **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 2.37 (s, 3H, *p*-CH_3), 2.43 (s, 6H, *o*-CH_3), 7.10 (s, 2H, Mes); **IR** (KBr) ν_{max}/cm^{-1} = 2964 w (CH), 2919 w (CH), 2850 w (CH), 2088 m (CO), 2051 s (CO), 2014 sh (CO), 1998 sh (CO), 1954 vs (CO), 1935 vs (CO); **MS** (EI, 70eV): m/z (%): 922.0 (2) [M$^+$], 722.9 (48) [As{W(CO)$_5$}$_2^+$], 694.8 (25) [As{W(CO)$_5$}$_2^+$-CO], 666.8 (48) [As{W(CO)$_5$}$_2^+$-2CO], 639.9 (87) [As{W(CO)$_5$}$_2^+$-3CO]; **elemental analysis** calcd. (%) for $C_{16}H_5AsO_{10}SW_2$: C 24.78, H 1.20; found: C 25.77, H 1.31.

^{1}H NMR spectrum:

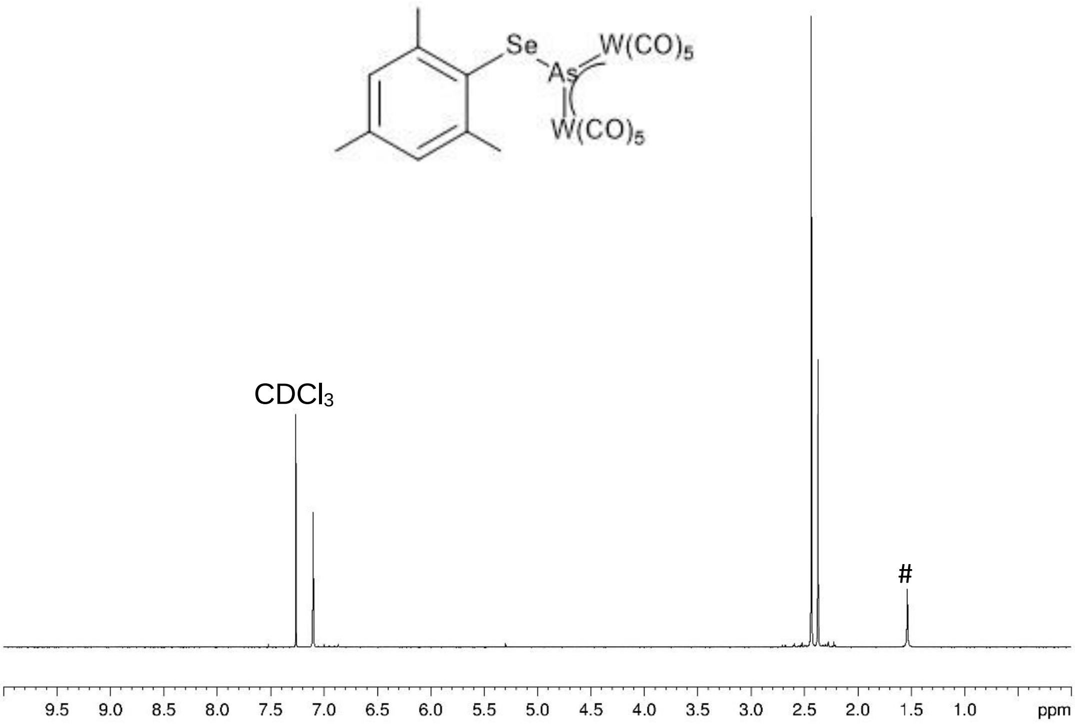


Figure S14. ^{1}H NMR spectrum of **3b** in $CDCl_3$. # = H_2O

2.6 Reaction of 1a with Ph_2Se_2

A solution of Ph_2Se_2 (36 mg, 0.2 mmol) in 10 mL toluene was added dropwise to a solution of **1a** (163 mg, 0.2 mmol) in 20 mL toluene at -80 °C. The solution is warmed to room temperature and stirred for 3 d, whereupon the blue solution turns brown. After analyzing the reaction solution via $^{31}P\{^1H\}$ NMR spectroscopy, it was purified via column chromatography (ø = 2.5 cm, l = 10 cm) using hexane/toluene in a 2:1 ratio. $[PhSeW(CO)_4]_2$ (**5)** crystallizes from the first of three fractions as green needles. Yield: 4 mg (2%)

5:^{1}H-NMR (CD_2Cl_2): δ = 7.31 (m, 6*H*, CH), 7.46 (m, 4*H*, CH).

Reaction solution:
$^{31}P\{^1H\}$ NMR ($CDCl_3$, 162 MHz): δ = 41.0 (s, $^1J_{P,W}$ = 275 Hz, 305 Hz $^1J_{P,Se}$ = 580 Hz, 607 Hz);
^{31}P NMR ($CDCl_3$, 162 MHz): δ = 41.0 (s, $^1J_{P,W}$ = 277 Hz, 303 Hz $^1J_{P,Se}$ = 582 Hz, 610 Hz)

$^{31}P\{^1H\}$ NMR of the reaction solution:

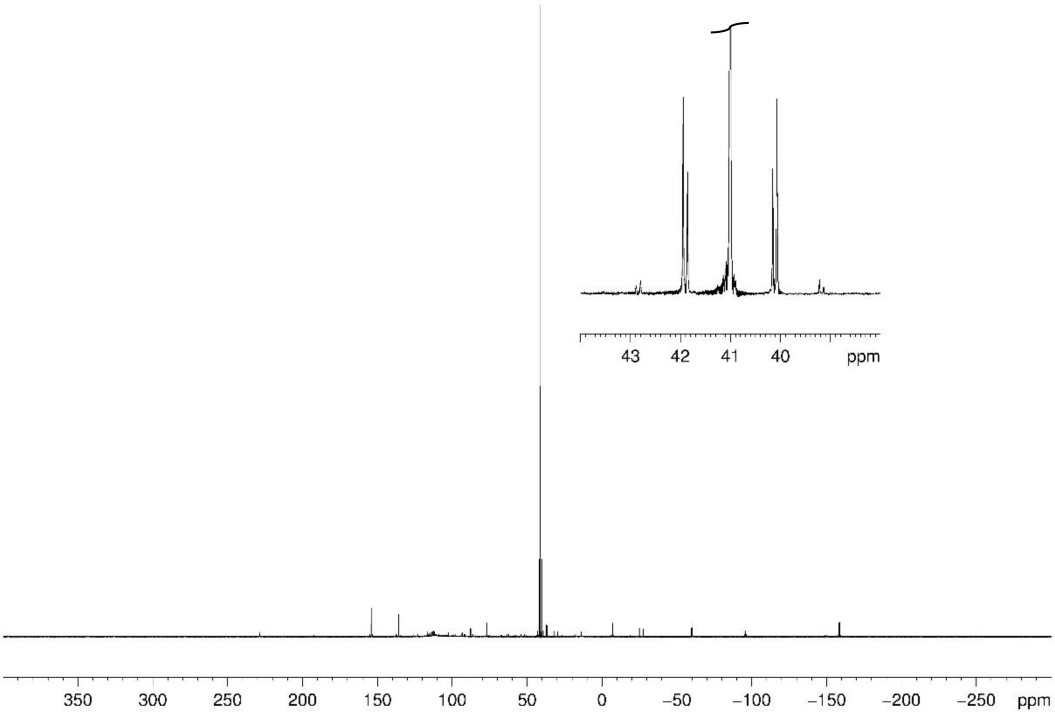


Figure S15. $^{31}P\{^1H\}$ NMR spectrum of the reaction solution of **1a** + Ph_2Se_2 in $CDCl_3$.

2.7 Reaction of 1a and Mes_2Te_2

A solution of Mes_2Te_2 (50 mg, 0.1 mmol) in 10 mL of toluene is added dropwise to a solution of **1a** (82 mg, 0.1 mmol) in 20 mL of toluene at -80 °C. The reaction mixture is stirred for 16 h and warmed to room temperature, whereupon the blue solution turns red. Before the solvent is removed in vacuo, the solution is analysed spectroscopically. $[Mes(W\{CO\}_5)Te]_2$ (**6a**) crystallizes from a concentrated CH_2Cl_2 solution at -28 °C as dark red blocks.

Yield: 6 mg (3%); **^{1}H NMR** (CD_2Cl_2, 400 MHz): δ = 2.35 (s, 6*H*, *p*-CH_3), 2.44 (s, 12*H*, *o*-CH_3), 6.97 (s, 4*H*, C_6H_2).

Photolytic reaction: A solution of Mes_2Te_2 (100 mg, 0.2 mmol) and **1a** (163 mg, 0.2 mmol) in 50 mL of toluene was irradiated for 20 min at 254 nm. The resulting violet solution was then characterized spectroscopically, wherein $[MesTeP\{W(CO)_5\}_2\}]$ (**4a-I**) could be identified.

^{31}P{^{1}H} NMR (C_6D_6, 162 MHz): δ = 122.2 (s), 840.4 (s, $^1J_{P,W}$ = 174 Hz, **4a-I**).

^{1}H NMR spectrum of the reaction solution (Photolytic reaction):

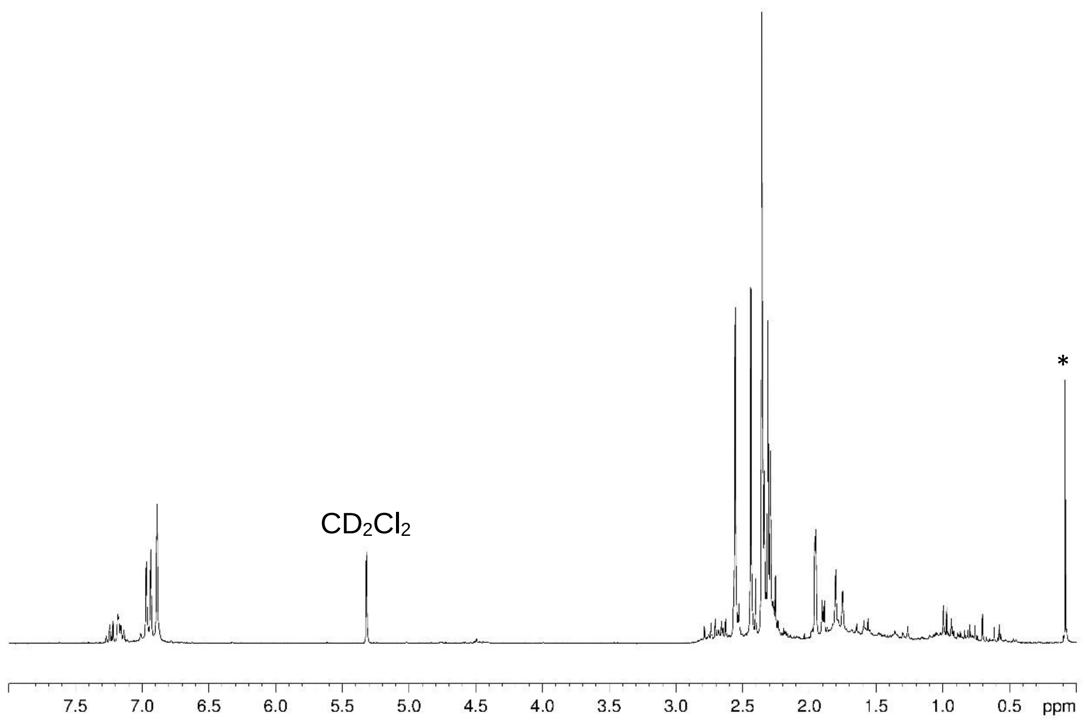


Figure S16. ^{1}H NMR spectrum of the reaction solution of **1a** + Mes_2Te_2 in CD_2Cl_2.* = grease.

$^{31}P\{^{1}H\}$ NMR spectra of the reaction solution (Photolytic reaction):

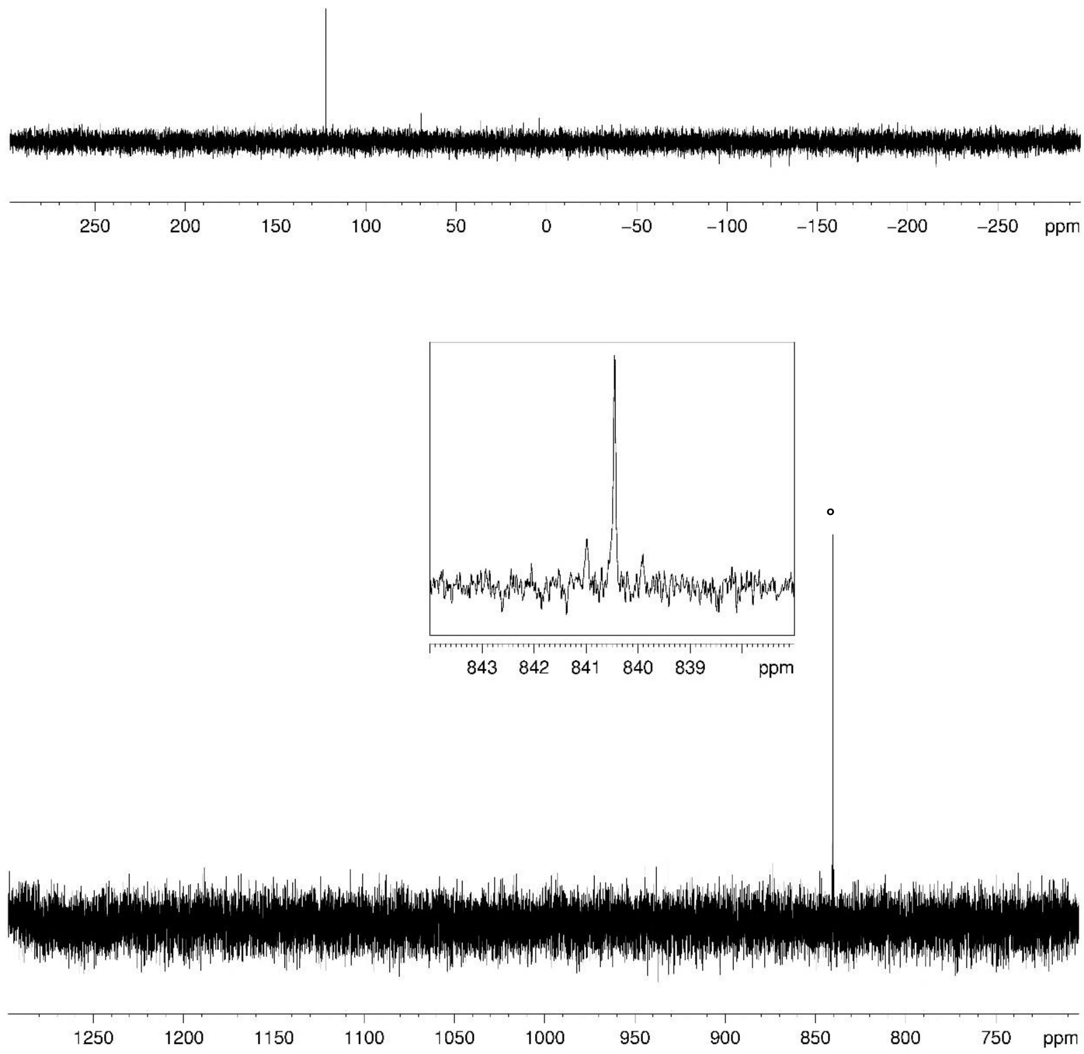


Figure S17. $^{31}P\{^{1}H\}$ NMR spectra of the reaction mixture of **1a** + Mes_2Te_2 in CD_2Cl_2. ° = **4a-I.**

2.8 Reaction of 1b and Mes_2Te_2

A mixture of **1b** (172 mg, 0.2 mmol) and Mes_2Te_2 (100 mg, 0.2 mmol) in 50 mL of toluene was irradiated for 20 minutes at 254 nm until the reaction solution turned a reddish violet. The solvent was removed and the residue extracted with hexane. [Mes(W{CO}$_5$)TeTeMes] (**6b**) was obtained from a concentrated solution at -28 °C as violet plates. Yield: few crystals.

6b: ^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 2.27 (s, 2H, CH_3), 2.44 (s, 2H, CH_3), 2,56 (s, 1H, CH_3), 2.81 (s, 4H, CH_3), 6.93 (s, 2H, CH).

^{1}H NMR spectrum of the reaction solution:

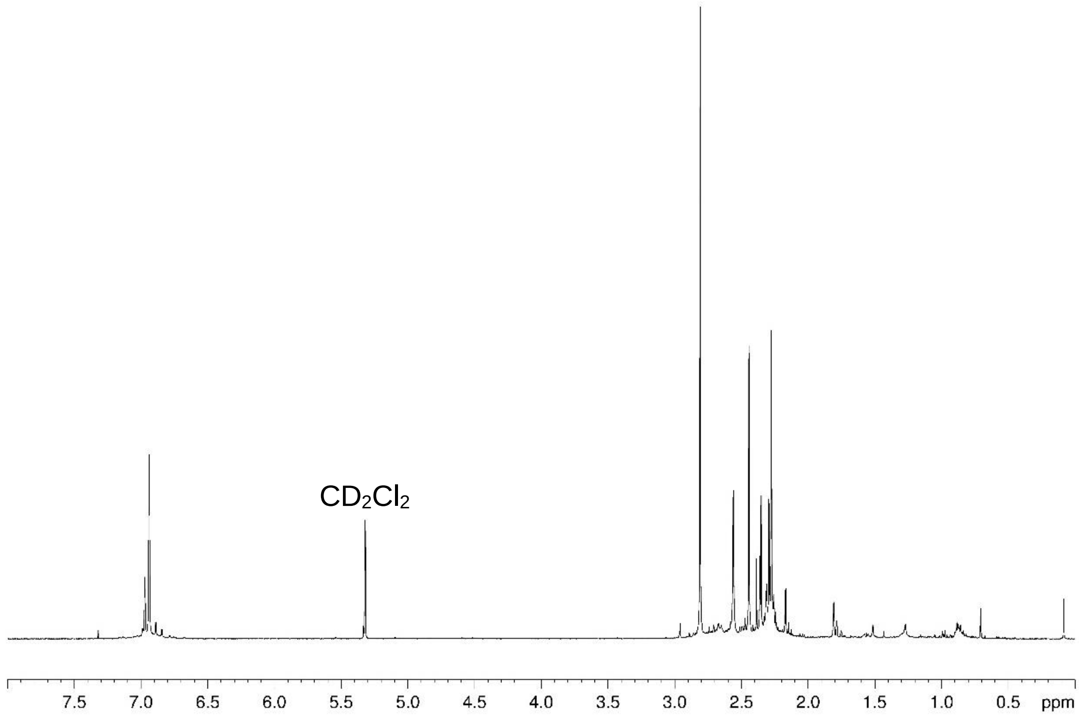


Figure S18. ^{1}H NMR spectrum of the reaction mixture of **1b** + Mes_2Te_2 in CD_2Cl_2.

2.9 Reaction of 1a with $Tipp_2Te_2$

A solution of $Tipp_2Te_2$ (132 mg, 0.2 mmol) and **1a** (163 mg, 0.2 mmol) in 50 mL of toluene was irradiated for 60 min at 254 nm. The resulting violet solution was then characterized spectroscopically, where [TippTeP{W(CO)$_5$}$_2$] (**4a-II**) could be identified.

4a-II: ^{31}P{^{1}H} NMR (CD_2Cl_2, 162 MHz): δ = 839 (s, $^1J_{P,W}$ = 174 Hz).

^{1}H NMR spectrum of the reaction solution:

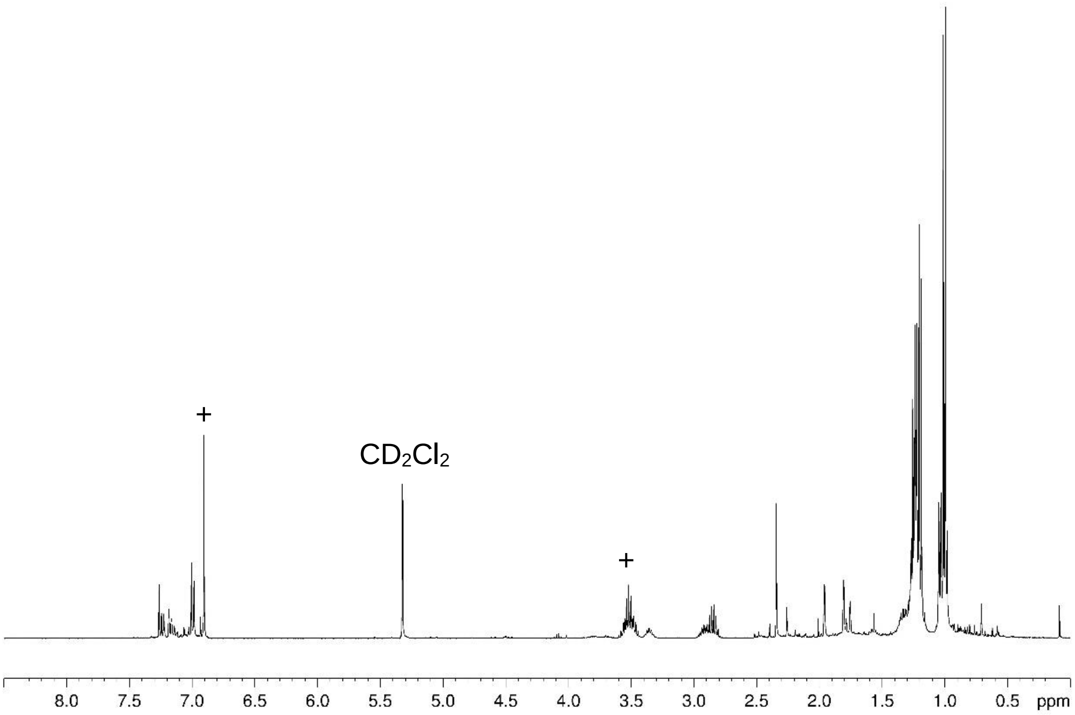


Figure S19. ^{1}H NMR spectrum of the reaction mixture of **1a** + $Tipp_2Te_2$ in CD_2Cl_2. **+ = $Tipp_2Te_2$**

^{31}P{^{1}H} NMR spectrum of the reaction solution:

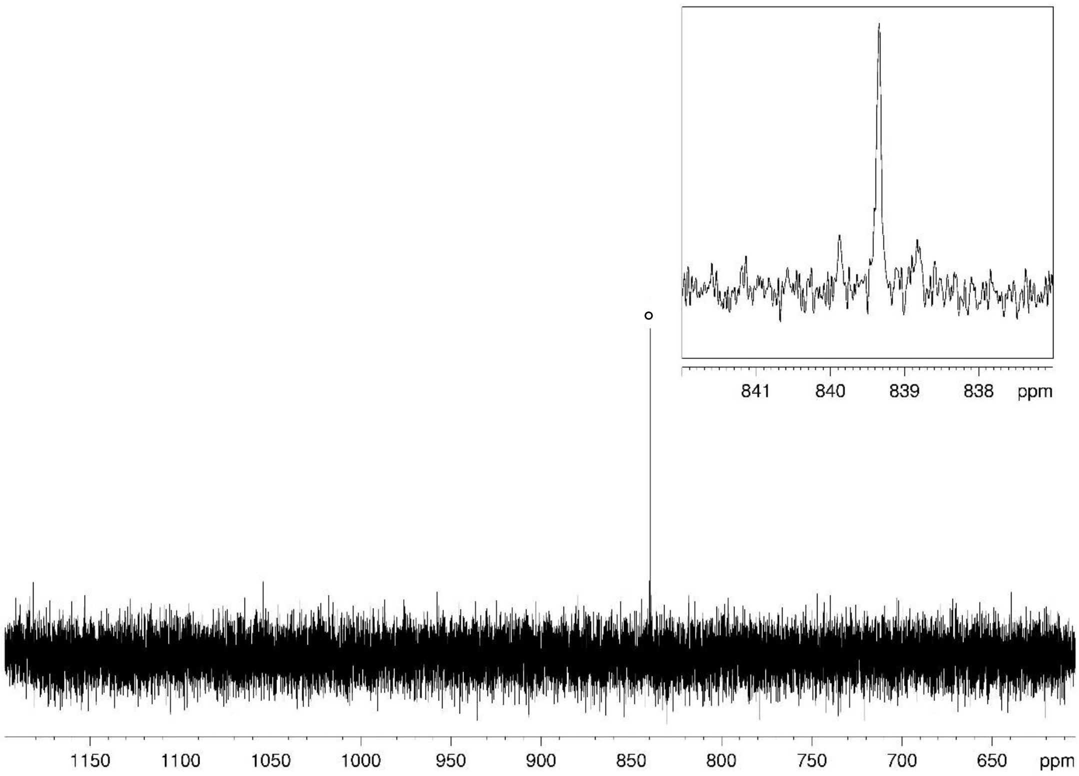


Figure S20. $^{31}P\{^{1}H\}$ NMR spectrum of the reaction mixture of **1a** + $Tipp_2Te_2$ in CD_2Cl_2. ° = **4a-II.**

3. Crystallographic Data

3.1. General information

Single crystal X-ray structure analyses were either carried out on a Gemini Ultra Diffractometer (Rigaku Oxford Diffraction, formerly Agilent Technologies) or a GV50 diffractometer (Rigaku Oxford Diffraction). The Gemini Ultra diffractometer was equipped with either a molybdenum X-ray radiation source (Mo-K_α = 0.71072 Å) or a copper X-ray radiation source (Cu-K_α = 1.5406 Å) and an AtlasS2 CCD detector as well as an Oxford Systems CryoJet cooling system. The GV50 diffractometer was equipped with a copper X-ray radiation source and a TitanS2 detector as well as an Oxford Cryosystems CryoStream 700 cooling system.

Figures of the molecular structures were prepared with the program *Olex2*[5].

CIF files with comprehensive information on the details of the diffraction experiments and full tables of bond lengths and angles for **2a**, **2b**, **3a-I**, **3a-II**, **3b**, **5**, **6a**, and **6b** are deposited in Cambridge Crystallographic Data Centre under the deposition codes CCDC-2083565, CCDC-2083566, CCDC-2083567, CCDC-2083568, CCDC-2083569, CCDC-2083570, CCDC-2083571, CCDC-2083572, respectively.

3.1.2. Handling

Due to their air and water sensitivity, the crystals were coated with mineral oil (Sigma Aldrich, CAS 8042-47-5). Suitable single crystals were picked under the microscope from the oil and transferred onto a MiTeGen MicroLoop attached to a goniometer head. The goniometer head was then placed onto the goniometer with the loop sitting in a current of cold nitrogen.

3.1.3. Data processing

After collection of the crystal structure data, integration and data reduction were carried out with the program *CrysAlis Pro*[6].

3.1.4. Structure solution and refinement

Structure elucidation was carried out with the program *SHELXT*[7] using direct methods. Refinement occurred with the least squares method with the program *SHELXL*[8]. Both were used within *Olex2*[5] as the platform.

3.2. Crystal Structure Data for compounds 2a, 2b, 3a-I, 3a-II, 3b

	2a	**2b**	**3a-I**	**3a-II**	**3b**
Formula	$C_{16}H_5O_{10}PSW_2$	$C_{16}H_5AsO_{10}SW_2$	$C_{16}H_5O_{10}PSeW_2$	$C_{38}H_{22}O_{20}P_2Se_2W_4$	$C_{38}H_{22}As_2O_{20}Se_2W_4$
$D_{calc.}$/ g cm^{-3}	2.486	2.632	2.637	2.436	2.520
m/mm^{-1}	22.032	23.124	23.108	20.365	20.952
Formula Weight	787.93	831.88	834.83	1753.81	1841.71
Colour	green	violet	dark red	metallic dark green	metallic dark green
Shape	block	needle	plate	block	block
Size/mm^3	0.18×0.07×0.06	0.21×0.04×0.02	0.14×0.11×0.03	0.60×0.33×0.28	0.49×0.33×0.19
T/K	123(1)	123.00(14)	123(2)	123.00(14)	123.2(4)
Crystal System	triclinic	monoclinic	monoclinic	triclinic	triclinic
Space Group	*P*-1	$P2_1/c$	$P2_1/c$	*P*-1	*P*-1
a/Å	6.59340(10)	6.97820(10)	7.01510(10)	9.61900(10)	9.7509(2)
b/Å	17.2561(4)	16.3547(2)	16.4460(2)	15.3701(2)	15.2808(5)
c/Å	19.7432(4)	18.6493(3)	18.4907(2)	18.5803(3)	18.6934(7)
a/°	109.413(2)	90	90	66.5430(10)	66.459(3)
b/°	91.241(2)	99.533(2)	99.7400(10)	78.3160(10)	78.315(2)
g/°	95.635(2)	90	90	72.3750(10)	72.751(2)
V/Å^3	2104.83(8)	2098.98(5)	2102.53(5)	2391.12(6)	2427.41(14)
Z	4	4	4	2	2
Z'	2	1	1	1	1
Wavelength/Å	1.54184	1.54184	1.54184	1.54184	1.54184
Radiation type	Cu K_a	Cu K_α	Cu K_α	Cu K_α	Cu K_α
Q_{min}/°	2.958	3.617	3.620	3.235	3.250
Q_{max}/°	73.827	66.815	72.061	66.589	74.127
Measured Refl's.	13300	16040	22306	29701	24588
Indep't Refl's	7859	3697	4109	8372	9207
Refl's I≥2 *s*(I)	7270	3472	3879	8226	8822
R_{int}	0.0284	0.0295	0.0454	0.0438	0.0475
Parameters	541	271	271	602	602
Restraints	0	0	0	0	0
Largest Peak	0.704	0.568	2.537	1.330	1.655
Deepest Hole	-0.800	-0.595	-1.009	-2.630	-2.108
GooF	1.005	1.053	1.096	1.224	1.193
wR_2 (all data)	0.0499	0.0360	0.0735	0.0842	0.0935
wR_2	0.0486	0.0352	0.0720	0.0837	0.0924
R_1 (all data)	0.0245	0.0184	0.0294	0.0323	0.0384
R_1	0.0220	0.0163	0.0275	0.0316	0.0366
Molecules in asymm. unit	1	1	1	2	2

3.3. Crystal Structure Data for compounds 5, 6a, 6b

	5	**6a**	**6b**
Formula	$C_{20}H_{10}O_8Se_2W_2$	$C_{28}H_{22}O_{10}Te_2W_2$	$C_{23}H_{22}O_5Te_2W$
$D_{calc.}$/ g cm^{-3}	2.718	2.342	2.143
μ/mm^{-1}	23.147	8.918	26.511
Formula Weight	903.90	1141.35	817.45
Colour	green	clear dark red	light violet
Shape	needle	block	plate
Size/mm^3	0.13×0.04×0.03	0.22×0.17×0.12	0.32×0.21×0.05
T/K	123.00(14)	123.00(14)	123
Crystal System	monoclinic	monoclinic	monoclinic
Space Group	$C2/c$	$P2_1/c$	$P2_1/c$
a/Å	18.3332(5)	9.9217(2)	16.5396(12)
b/Å	7.2060(2)	12.1683(2)	18.5800(3)
c/Å	17.1601(5)	13.7521(2)	28.924(2)
α/°	90	90	90
β/°	102.976(4)	102.838(2)	145.249(17)
γ/°	90	90	90
V/Å^3	2209.11(11)	1618.79(5)	5066.6(13)
Z	4	2	8
Z'	0.5	0.5	2
Wavelength/Å	1.54184	0.71073	1.54184
Radiation type	Cu K_α	Mo K_α	Cu K_α
Θ_{min}/°	4.951	2.850	3.584
Θ_{max}/°	73.958	29.431	72.941
Measured Refl's.	4009	30810	27607
Indep't Refl's	2077	4243	9821
Refl's I≥2 σ(I)	1852	4027	9047
R_{int}	0.0573	0.0309	0.0351
Parameters	145	193	571
Restraints	0	0	0
Largest Peak	1.626	0.897	1.427
Deepest Hole	-1.469	-0.590	-1.143
GooF	1.054	1.071	1.097
wR_2 (all data)	0.1019	0.0374	0.0776
wR_2	0.0978	0.0367	0.0756
R_1 (all data)	0.0392	0.0192	0.0337
R_1	0.0351	0.0175	0.0296
Molecules in asymm. unit	1	1	2

3.4. Bonds, angles and figures for the crystal structures

*3.4.1. [PhSP{W(CO)$_5$}$_2$] (**2a**)*

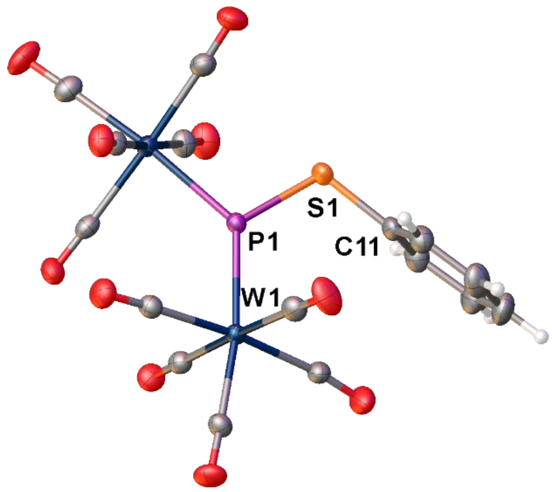


Figure S21. Molecular structure of **2a**. Anisotropic displacement parameters are set to 50% probability level. Selected bond lengths [Å] and angles [°]: W1-P1 2.4065(9), W2-P1 2.4239(9), P1-S1 2.0703(13), S1-C11 1.787(4); W1-P1-W2 132.12(4), S1-P1-W2 104.68(4), S1-P1-W1 123.17(5), C11-S1-P1 109.59(13).

*3.4.2. [PhSAs{W(CO)$_5$}$_2$] (**2b**)*

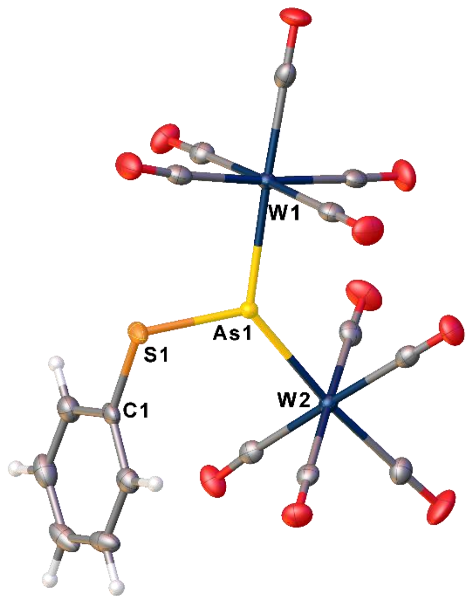


Figure S22. Molecular structure of **2b**. Anisotropic displacement parameters are set to 50% probability level. Selected bond lengths [Å] and angles [°]: W1-As1 2.5024(3), W2-As1 2.5043(3), As1-S1 2.1958(8), S1-C1 1.776(3); W1-As1-W2 133.550(14), S1-As1-W1 104.62(2), S1-As1-W2 121.82(2), C1-S1-As1 108.61(10).

*3.4.3. [PhSeP{W(C)O)₅}₂] (**3a-I**)*

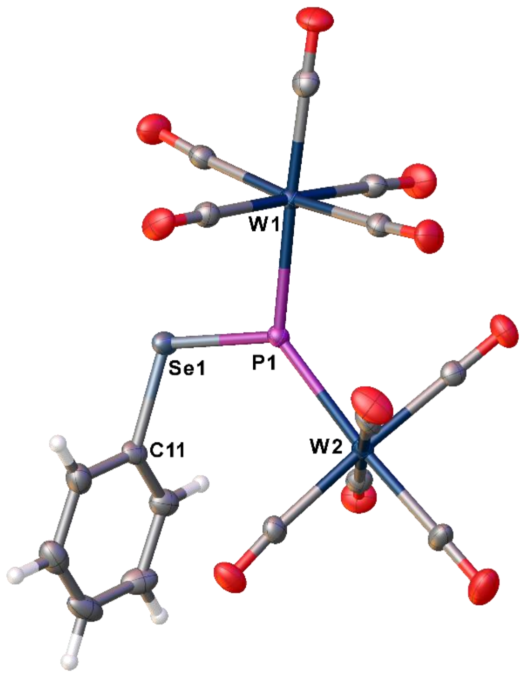


Figure S23. Molecular structure of **3a-I**. Anisotropic displacement parameters are set to 50% probability level. Selected bond lengths [Å] and angles [°]: W1-P1 2.4232(11), W2-P1 2.4141(11), Se1-P1 2.2060(13), Se1-C11 1.925(5); W2-P1-W1 132.95(5), Se1-P1-W1 104.19(4), Se1-P1-W2 122.84(5), C11-Se1-P1 107.95(14).

*3.4.4. [MesSeP{W(CO)₅}₂] (**3a-II**)*

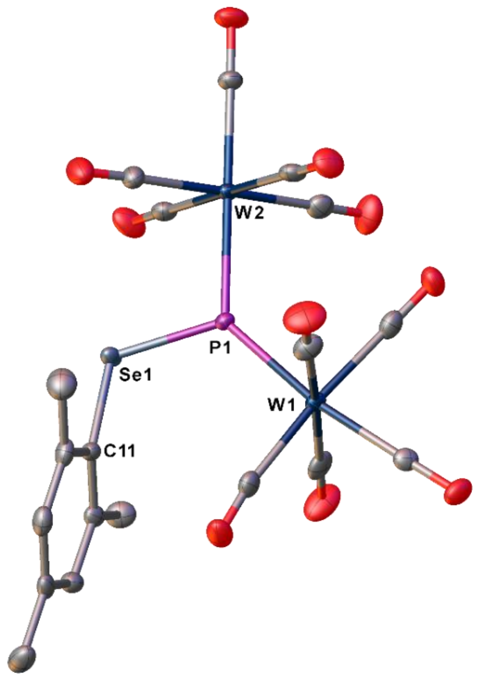


Figure S24. Molecular structure of **3a-II**. Anisotropic displacement parameters are set to 50% probability level. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: W1-P1 2.4134(11), W2-P1 2.4360(11), Se1-P1 2.1974(13), Se1-C11 1.924(4); W1-P1-W2 133.23(5), Se1-P1-W2 103.50(5), Se1-P1-W1 123.27(5).

*3.4.5. [MesSeAs{W(CO)$_5$}$_2$] (**3b**)*

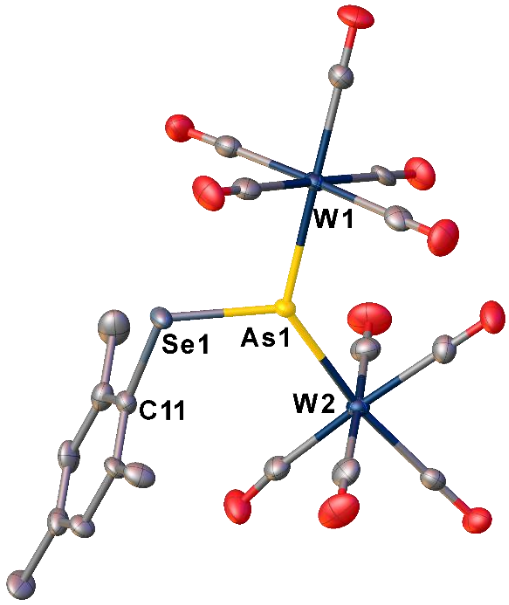


Figure S25. Molecular structure of **3b**. Anisotropic displacement parameters are set to 50% probability level. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: W1-As1 2.5192(6), W2-As1 2.5024(6), As1-Se1 2.3193(8), Se1-C11 1.910(6); W2-As1-W1 133.83(3), Se1-As1-W1 103.28(2), Se1-As1-W2 122.86(3), C11-Se1-As1 108.23(16).

*3.4.7. [PhSe{W(CO)$_4$}]$_2$ (**5**)*

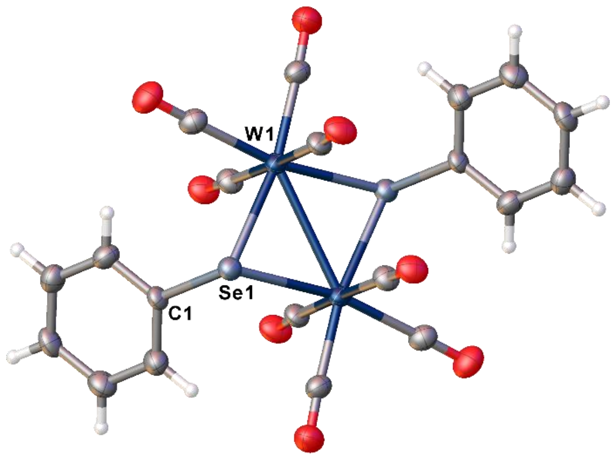


Figure S26. Molecular structure of **5**. Anisotropic displacement parameters are set to 50% probability level. Selected bond lengths [Å] and angles [°]: W1-W1[2] 3.0247(6), W1-Se1 2.5891(8), W1-Se1[2] 2.5929(8), Se1-C1 1.953(7); Se1[2]-W1-W1[2] 54.231(19), Se1-W1-W1[2] 54.347(19), Se1-W1-Se1[2] 108.58(2), W1-Se1-W1[2] 74.42(2), C1-Se1-W1[2] 107.8(2), C1-Se1-W1 110.1(2).

[2] 1-x, 1-y, 1-z

*3.4.9. [Mes(W{CO}$_5$)Te]$_2$ (**6a**)*

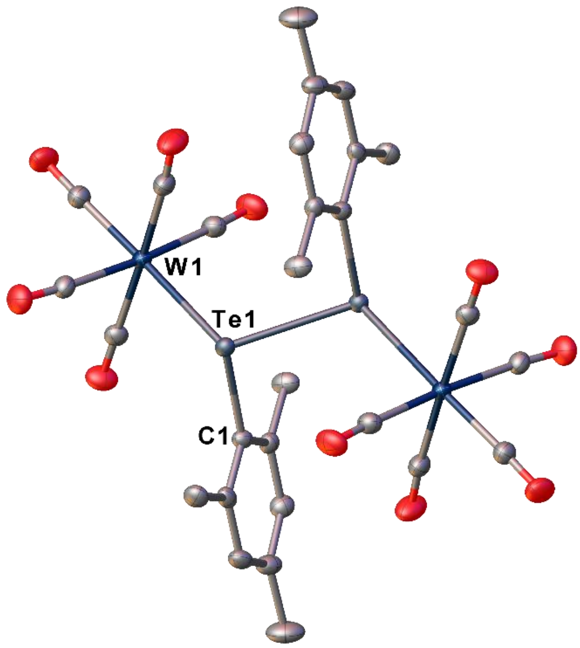


Figure S27. Molecular structure of **6a**. Anisotropic displacement parameters are set to 50% probability level. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: W1-Te1 2.79539(17), Te1-Te1[3] 2.8186(3), Te1-C1 2.139(2); W1-Te1-Te1[3] 108.710(8), C1-Te1-W1 112.93(6), C1-Te1-Te1[3] 94.27(7).

*3.4.10. [Mes(W{CO}$_5$)TeTeMes] (**6b**)*

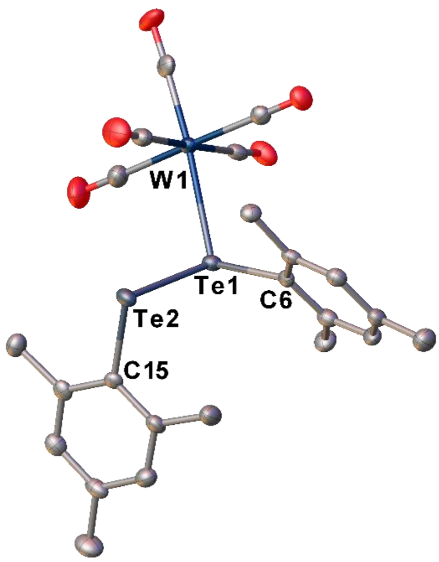


Figure S28. Molecular structure of **6b**. Anisotropic displacement parameters are set to 50% probability level. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: W1-Te1 2.8145(5), Te1-Te2 2.7574(11), Te1-C6 2.145(4), Te2-C15 2.126; Te2-Te1-W1 105.09(2), C6-Te1-W1 115.23(11), C6-Te1-Te2 99.57(11), C15-Te2-Te1 95.63(11).

[3] 1-x, 1-y, 1-z

4. 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[9] with def2-SVPD all electron basis set (ECP on W).[10] Gaussian 16 program package[11] was used throughout. All structures correspond to minima on their respective potential energy surfaces as verified by computation of second derivatives. Basis sets were obtained from the EMSL basis set exchange database.[12]

Gas phase chemical shifts were calculated at PBE0[13] level of theory both on experimental and optimized geometries using GIAO approach[14]. Chemical shifts of phosphorus nuclei are given relative to the H_3PO_4 optimized in the gas phase. Values are scaled by the linear equation recommended by *Sinyashin et al.*[15]: $\delta_{scaled}=(\delta_{unscaled}-a)/k$, where values of a=14.4 and k=1.073 were obtained at PBE/6-311G(2d,2p) level of theory by fitting known ^{31}P chemical shifts of 34 organophosphorus compounds.

Standard entropies of the reactions in solution were estimated by taking into account the entropy of the solvation of one gaseous mole in the inert solvent (90 J mol^{-1} K^{-1}).[16]

Table S1. Experimental and computed ^{31}P NMR chemical shifts, on gas phase optimized and on experimental geometries (ppm). All computed chemical shifts are scaled according to [15].

	Exp.	PBE0/def2-SVPD		PBE0/6-311++G(2d,2p)// PBE0/def2-SVPD
Compound		on optimized geom.	on exp. geom.	on optimized geom.
PhSP{W(CO)$_5$}	822.9	866.2	809.7	927.6
PhSeP{W(CO)$_5$}	835.0	898.3	869.1	966.9
MesSeP{W(CO)$_5$}	854.3	911.9	873.5	991.5
MesTeP{W(CO)$_5$}	840.4	958.8		1044.9

Table S2. Gas phase reaction energies ΔE°$_0$, enthalpiesΔH°$_{298}$, Gibbs energies ΔG°$_{298}$ in kJ mol^{-1}, and reaction entropies ΔS°$_{298}$, J mol^{-1} K^{-1}. B3LYP/def2-SVPD (ECP on W) level of theory. Reaction entropies and Gibbs energies in solution were estimated according to [16].

Reaction	ΔE°$_0$	ΔH°$_{298}$	ΔS°$_{298}$	ΔG°$_{298}$	ΔS°$_{298}$ solvent	ΔG°$_{298}$ solvent
Cp*P{W(CO)$_5$}$_2$ = Cp* +P{W(CO)$_5$}$_2$	128.7	114.6	293.0	27.3	203.0	54.1
(Cp*)$_2$ = 2 Cp*	111.4	87.3	300.6	-2.3	210.6	24.6
Ph$_2$S$_2$ = 2 PhS	165.0	157.6	159.9	109.9	69.9	136.7
Ph$_2$Se$_2$ = 2 PhSe	225.4	219.2	159.2	171.7	69.2	198.6
Ph$_2$Te$_2$ = 2 PhTe	164.3	158.8	152.9	113.2	62.9	140.1
Mes$_2$S$_2$ = 2 MesS	130.9	123.7	156.8	76.9	66.8	103.8
Mes$_2$Se$_2$ = 2 MesSe	189.6	182.6	153.9	136.7	63.9	163.5
Mes$_2$Te$_2$ = 2 MesTe	144.9	138.8	158.1	91.7	68.1	118.5
Cp*P{W(CO)$_5$}$_2$ + ½ Ph$_2$S$_2$ = Cp* + PhSP{W(CO)$_5$}$_2$	1.4	-8.9	139.9	-50.6	94.9	-37.2
Cp*P{W(CO)$_5$}$_2$ + ½ Ph$_2$Se$_2$ = Cp* + PhSeP{W(CO)$_5$}$_2$	15.2	4.6	142.8	-38.0	97.8	-24.6
Cp*P{W(CO)$_5$}$_2$ + ½ Ph$_2$Te$_2$ = Cp* + PhTeP{W(CO)$_5$}$_2$	34.0	22.8	148.7	-21.5	103.7	-8.1
Cp*P{W(CO)$_5$}$_2$ + ½ Mes$_2$S$_2$ = Cp* + MesSP{W(CO)$_5$}$_2$	-9.9	-20.0	132.3	-59.4	87.3	-46.0
Cp*P{W(CO)$_5$}$_2$ + ½ Mes$_2$Se$_2$ = Cp* + MesSeP{W(CO)$_5$}$_2$	5.0	-5.6	152.5	-51.0	107.5	-37.6
Cp*P{W(CO)$_5$}$_2$ + ½ Mes$_2$Te$_2$ = Cp* + MesTeP{W(CO)$_5$}$_2$	24.3	13.3	146.0	-30.3	101.0	-16.9
P{W(CO)$_5$}$_2$ + Ph$_2$S$_2$ = PhS + PhSP{W(CO)$_5$}$_2$	-44.8	-44.7	-73.1	-22.9	-73.1	-22.9
P{W(CO)$_5$}$_2$ + Ph$_2$Se$_2$ = PhSe + PhSeP{W(CO)$_5$}$_2$	-0.8	-0.4	-70.6	20.6	-70.6	20.6
P{W(CO)$_5$}$_2$ + Ph$_2$Te$_2$ = PhTe + PhTeP{W(CO)$_5$}$_2$	-12.6	-12.4	-67.8	7.8	-67.8	7.8
P{W(CO)$_5$}$_2$ + Mes$_2$S$_2$ = MesS + MesSP{W(CO)$_5$}$_2$	-73.2	-72.8	-82.3	-48.2	-82.3	-48.2
P{W(CO)$_5$}$_2$ + Mes$_2$Se$_2$ = MesSe + MesSeP{W(CO)$_5$}$_2$	-28.9	-28.9	-63.5	-9.9	-63.5	-9.9
P{W(CO)$_5$}$_2$ + Mes$_2$Te$_2$ = MesTe + MesTeP{W(CO)$_5$}$_2$	-32.0	-31.9	-67.9	-11.7	-67.9	-11.7
Cp*P{W(CO)$_5$}$_2$ + PhSH = HCp* + PhSP{W(CO)$_5$}$_2$	-84.5	-79.4	25.6	-87.0	25.6	-87.0
Cp*P{W(CO)$_5$}$_2$ + PhSeH = HCp* + PhSeP{W(CO)$_5$}$_2$	-96.2	-89.7	14.7	-94.0	14.7	-94.0
Cp*P{W(CO)$_5$}$_2$ + PhTeH = HCp* + PhTeP{W(CO)$_5$}$_2$	-106.3	-97.7	30.0	-106.7	30.0	-106.7
Cp*P{W(CO)$_5$}$_2$ + MesSH = HCp* + MesSP{W(CO)$_5$}$_2$	-86.7	-81.8	22.0	-88.4	22.0	-88.4
Cp*P{W(CO)$_5$}$_2$ + MesSeH = HCp* + MesSeP{W(CO)$_5$}$_2$	-95.3	-88.9	38.9	-100.5	38.9	-100.5
Cp*P{W(CO)$_5$}$_2$ + MesTeH = HCp* + MesTeP{W(CO)$_5$}$_2$	-104.1	-95.5	27.5	-103.7	27.5	-103.7
Cp*P{W(CO)$_5$}$_2$ + PhSH = Cp*P{W(CO)$_5$}$_2$·PhSH	37.7	44.2	-220.0	109.8	-130.0	83.0
Cp*P{W(CO)$_5$}$_2$ + PhSeH = Cp*P{W(CO)$_5$}$_2$·PhSeH	34.9	40.5	-227.0	108.2	-137.0	81.4
Cp*P{W(CO)$_5$}$_2$ + PhTeH = Cp*P{W(CO)$_5$}$_2$·PhTeH	33.2	38.8	-212.4	102.1	-122.4	75.3
Cp*P{W(CO)$_5$}$_2$ + PhS = Cp*P{W(CO)$_5$}$_2$·PhS	-55.7	-48.7	-194.4	9.3	-104.4	-17.5
Cp*P{W(CO)$_5$}$_2$ + PhSe = Cp*P{W(CO)$_5$}$_2$·PhSe	-76.7	-70.4	-197.6	-11.5	-107.6	-38.3
Cp*P{W(CO)$_5$}$_2$ + PhTe = Cp*P{W(CO)$_5$}$_2$·PhTe	-35.7	-30.2	-199.3	29.2	-109.3	2.4
Cp*P{W(CO)$_5$}$_2$·PhSH = Cp*H + PhSP{W(CO)$_5$}$_2$	-122.2	-123.6	245.5	-196.8	155.5	-170.0
Cp*P{W(CO)$_5$}$_2$·PhSeH = Cp*H + PhSeP{W(CO)$_5$}$_2$	-131.1	-130.2	241.7	-202.2	151.7	-175.4
Cp*P{W(CO)$_5$}$_2$·PhTeH = Cp*H + PhTeP{W(CO)$_5$}$_2$	-139.5	-136.5	242.3	-208.8	152.3	-181.9
Cp*P{W(CO)$_5$}$_2$·PhS = Cp* + PhSP{W(CO)$_5$}$_2$	-25.4	-39.0	254.4	-114.8	164.4	-88.0
Cp*P{W(CO)$_5$}$_2$·PhSe = Cp* + PhSeP{W(CO)$_5$}$_2$	-20.8	-34.6	260.7	-112.4	170.7	-85.5
Cp*P{W(CO)$_5$}$_2$·PhTe = Cp* + PhTeP{W(CO)$_5$}$_2$	-12.4	-26.4	271.5	-107.4	181.5	-80.5
Cp*P{W(CO)$_5$}$_2$ + Ph$_2$S$_2$ = Cp* + PhS + PhSP{W(CO)$_5$}$_2$	83.9	69.9	219.9	4.4	129.9	31.2
Cp *P{W(CO)$_5$}$_2$ + Ph$_2$Se$_2$ = Cp* + PhSe + PhSeP{W(CO)$_5$}$_2$	127.9	114.2	222.4	47.9	132.4	74.7
Cp *P{W(CO)$_5$}$_2$ + Ph$_2$Te$_2$ = Cp* + PhTe + PhTeP{W(CO)$_5$}$_2$	116.1	102.2	225.2	35.1	135.2	61.9

Table S3. Total energies E^o_0, sum of electronic and thermal enthalpies H^o_{298} (Hartree) and standard entropies S^o_{298} (cal mol^{-1}K^{-1}) for studied compounds. B3LYP/def2-SVPD (ECP on W) level of theory.

Compound	E^o_0	H^o_{298}	S^o_{298}
Cp*P{W(CO)$_5$}$_2$	-1998.074106	-1997.726543	255.279
P{W(CO)$_5$}$_2$	-1608.222862	-1608.110192	211.186
Cp*	-389.8022192	-389.572698	114.119
HCp*	-390.4336937	-390.190214	107.606
(Cp*)$_2$	-779.646884	-779.178663	156.397
Ph_2S_2	-1259.167212	-1258.970067	116.934
Ph_2Se_2	-5265.593876	-5265.397772	123.375
Ph_2Te_2	-999.2120126	-999.016188	128.912
PhS	-629.5521767	-629.455028	77.571
PhSe	-2632.754012	-2632.657141	80.716
PhTe	-499.5747193	-499.477846	82.729
PhSH	-630.1823598	-630.075681	79.286
PhSeH	-2633.385984	-2633.28051	85.794
PhTeH	-500.1840423	-500.079707	86.315
PhSP{W(CO)$_5$}$_2$	-2237.854952	-2237.642255	233.07
PhSeP{W(CO)$_5$}$_2$	-4241.063034	-4240.85099	236.973
PhTeP{W(CO)$_5$}$_2$	-2107.864944	-2107.653253	241.156
Mes_2S_2	-1494.906249	-1494.535302	165.612
Mes_2Se_2	-5501.330759	-5500.960724	172.102
Mes_2Te_2	-1234.945736	-1234.576189	175.936
MesS	-747.4281989	-747.244098	101.543
MesSe	-2750.629273	-2750.445586	104.447
MesTe	-617.4452823	-617.261661	106.867
MesSH	-748.0553572	-747.861612	102.642
MesSeH	-2751.258643	-2751.066128	106.682
MesTeH	-618.0554551	-617.864192	109.791
MesSP{W(CO)$_5$}$_2$	-2355.728791	-2355.429107	255.58
MesSeP{W(CO)$_5$}$_2$	-4358.935359	-4358.636331	263.659
MesTeP{W(CO)$_5$}$_2$	-2225.735511	-2225.436889	264.029
Cp*P{W(CO)$_5$}$_2$·SHPh	-2628.242112	-2627.785385	281.995
Cp*P{W(CO)$_5$}$_2$·SeHPh	-4631.446804	-4630.991622	286.816
Cp*P{W(CO)$_5$}$_2$·TeHPh	-2498.245498	-2497.791476	290.839
Cp*P{W(CO)$_5$}$_2$·SPh	-2627.647488	-2627.200101	286.392
Cp*P{W(CO)$_5$}$_2$·SePh	-4630.857325	-4630.410494	288.774
Cp*P{W(CO)$_5$}$_2$·TePh	-2497.662422	-2497.215882	290.386

Table S4. Optimized xyz coordinates (in Angstroms) for studied compounds. B3LYP/def2-SVPD (ECP on W) level of theory.

Cp*P{W(CO)$_5$}$_2$			
6	-0.684066000	3.352063000	0.405450000
6	0.455018000	2.350011000	0.173394000
6	1.205780000	2.632434000	-1.115337000
6	2.494840000	2.955701000	-0.797879000
6	2.681578000	2.870798000	0.658657000
6	1.509752000	2.493206000	1.245988000
15	-0.070974000	0.500883000	0.081462000
6	0.550896000	2.655382000	-2.464336000
6	3.585967000	3.394954000	-1.725439000
6	3.969872000	3.222748000	1.337205000
6	1.204918000	2.376195000	2.711046000
74	-2.544971000	0.032645000	0.007398000
74	1.741468000	-1.265582000	-0.013645000
6	3.066616000	-2.834546000	-0.087398000
6	0.335759000	-2.767304000	0.232249000
6	3.424322000	-0.076212000	-0.291847000
6	2.025151000	-1.116145000	2.050011000
6	1.511031000	-1.343155000	-2.090133000
6	-4.528145000	-0.534170000	-0.105257000
6	-2.295059000	-1.319178000	1.582690000
6	-2.904988000	1.415951000	-1.502734000
6	-2.156655000	-1.436581000	-1.419931000
6	-3.122014000	1.461029000	1.405651000
8	-1.997799000	-2.240242000	-2.221657000
8	-3.519321000	2.214129000	2.176212000
8	-2.195130000	-2.033321000	2.472675000
8	-5.628361000	-0.857756000	-0.173134000
8	-3.145537000	2.177432000	-2.328015000
8	1.405672000	-1.373897000	-3.231366000
8	2.203637000	-1.031328000	3.179758000
8	-0.344045000	-3.685179000	0.357139000
8	4.460328000	0.395027000	-0.458966000
8	3.801853000	-3.717996000	-0.127909000
1	-1.464532000	3.281238000	-0.357511000
1	-0.265869000	4.367993000	0.368317000
1	-1.147447000	3.216567000	1.387721000
1	0.815916000	3.325743000	3.115616000
1	2.097417000	2.119169000	3.293952000
1	0.446925000	1.609427000	2.918918000
1	4.229633000	4.279101000	1.162822000
1	4.804523000	2.623719000	0.943617000
1	3.920631000	3.068056000	2.420894000
1	3.261097000	3.412905000	-2.771328000
1	4.456462000	2.725775000	-1.654253000
1	3.941720000	4.403917000	-1.463497000
1	0.257277000	1.653562000	-2.812952000
1	1.219998000	3.075312000	-3.223942000
1	-0.363775000	3.267594000	-2.458204000
P{W(CO)$_5$}$_2$			
15	-0.000291000	0.440461000	0.001411000
74	-2.375095000	0.028871000	0.000826000
74	2.375440000	0.032232000	-0.000617000
6	4.418928000	-0.382960000	-0.002740000

6	1.951982000	-2.001753000	0.197169000
6	2.744614000	2.081994000	-0.196856000
6	2.467487000	0.227637000	2.084027000
6	2.384524000	-0.170695000	-2.086176000
6	-4.418157000	-0.389951000	-0.000240000
6	-2.133963000	-1.290198000	1.606384000
6	-2.655038000	1.350622000	-1.599687000
6	-2.065288000	-1.558196000	-1.323738000
6	-2.693794000	1.623085000	1.320113000
8	-1.892230000	-2.430618000	-2.044964000
8	-2.878196000	2.499341000	2.033692000
8	-2.001785000	-2.017025000	2.481061000
8	-5.537516000	-0.643481000	-0.000911000
8	-2.820051000	2.078899000	-2.467495000
8	2.398496000	-0.283784000	-3.224987000
8	2.529025000	0.335434000	3.221772000
8	1.709403000	-3.116021000	0.304961000
8	2.950452000	3.203592000	-0.302407000
8	5.538786000	-0.634591000	-0.003986000
Cp*			
6	-1.534586000	-2.230810000	0.004225000
6	-0.641235000	-1.031938000	0.001323000
6	0.733231000	-0.983291000	-0.001020000
6	1.113315000	0.422084000	-0.006617000
6	-0.070567000	1.233629000	-0.005963000
6	-1.153633000	0.366660000	-0.000709000
6	1.715034000	-2.116985000	-0.007538000
6	2.521708000	0.913690000	0.010339000
6	-0.082186000	2.735618000	-0.005754000
6	-2.609473000	0.700005000	0.003494000
1	3.007883000	0.688489000	0.976385000
1	2.586039000	1.996857000	-0.148504000
1	3.131210000	0.414022000	-0.760112000
1	2.417823000	-2.054420000	0.839967000
1	2.329373000	-2.123382000	-0.923943000
1	1.213030000	-3.090226000	0.055339000
1	-2.195395000	-2.241133000	0.887637000
1	-0.964956000	-3.167721000	0.003264000
1	-2.198143000	-2.242727000	-0.877149000
1	-3.121484000	0.273851000	-0.876119000
1	-2.787596000	1.781661000	0.003073000
1	-3.115679000	0.275937000	0.887437000
1	0.446788000	3.152568000	-0.878580000
1	0.406530000	3.152913000	0.890307000
1	-1.105072000	3.131339000	-0.029681000
HCp*			
6	-2.177334000	-0.168840000	1.547676000
6	-0.923028000	0.001191000	0.742513000
6	0.344451000	0.181032000	1.192198000
6	1.273091000	0.313096000	0.000000000
6	0.344451000	0.181032000	-1.192198000
6	-0.923028000	0.001191000	-0.742513000
6	0.841861000	0.264817000	2.601407000
1	1.701531000	1.335008000	0.000000000
6	2.438872000	-0.691345000	0.000000000
6	0.841861000	0.264817000	-2.601407000
6	-2.177334000	-0.168840000	-1.547676000

1	1.377636000	1.211700000	2.783623000
1	1.554775000	-0.544834000	2.832533000
1	0.025770000	0.200756000	3.331617000
1	-2.912900000	0.618375000	1.315248000
1	-1.983169000	-0.135925000	2.626031000
1	-2.668275000	-1.130241000	1.325314000
1	-2.912900000	0.618375000	-1.315248000
1	-2.668275000	-1.130241000	-1.325314000
1	-1.983169000	-0.135925000	-2.626031000
1	1.377636000	1.211700000	-2.783623000
1	0.025770000	0.200756000	-3.331617000
1	1.554775000	-0.544834000	-2.832533000
1	3.075102000	-0.560540000	0.886175000
1	3.075102000	-0.560540000	-0.886175000
1	2.057408000	-1.722478000	0.000000000

$(Cp^*)_2$

6	1.356004000	-2.356278000	1.978081000
6	0.458520000	-1.959929000	0.839164000
6	-1.197375000	-0.881196000	-0.503635000
6	-0.859820000	-2.069481000	-1.064910000
6	0.150225000	-2.741141000	-0.225972000
6	-1.399645000	-0.807460000	1.984816000
6	-2.233831000	0.079542000	-0.998517000
6	-1.399645000	-2.688347000	-2.321151000
6	0.687709000	-4.103514000	-0.552470000
1	-1.783839000	0.985943000	-1.426268000
1	-2.897817000	0.414819000	-0.187456000
1	-2.864728000	-0.379911000	-1.769238000
1	-2.213833000	-0.081301000	1.915756000
1	-0.903643000	-0.666046000	2.953609000
1	-1.843873000	-1.810799000	1.980039000
1	1.376622000	-3.446794000	2.101693000
1	1.023441000	-1.927181000	2.932467000
1	2.400456000	-2.035875000	1.835499000
1	1.384053000	-4.470233000	0.210056000
1	1.226022000	-4.097848000	-1.514077000
1	-0.123211000	-4.842001000	-0.654732000
1	-2.163754000	-2.063640000	-2.796732000
1	-1.847447000	-3.675409000	-2.123111000
1	-0.599319000	-2.851821000	-3.060753000
6	-0.407291000	-0.688546000	0.798469000
6	0.407291000	0.688546000	0.798469000
6	1.197375000	0.881196000	-0.503635000
6	0.859820000	2.069481000	-1.064910000
6	-0.150225000	2.741141000	-0.225972000
6	-0.458520000	1.959929000	0.839164000
6	1.399645000	0.807460000	1.984816000
6	2.233831000	-0.079542000	-0.998517000
6	1.399645000	2.688347000	-2.321151000
6	-0.687709000	4.103514000	-0.552470000
6	-1.356004000	2.356278000	1.978081000
1	2.213833000	0.081301000	1.915756000
1	0.903643000	0.666046000	2.953609000
1	1.843873000	1.810799000	1.980039000
1	-1.023441000	1.927181000	2.932467000
1	-2.400456000	2.035875000	1.835499000
1	-1.376622000	3.446794000	2.101693000

1	-1.226022000	4.097848000	-1.514077000
1	0.123211000	4.842001000	-0.654732000
1	-1.384053000	4.470233000	0.210056000
1	0.599319000	2.851821000	-3.060753000
1	2.163754000	2.063640000	-2.796732000
1	1.847447000	3.675409000	-2.123111000
1	2.864728000	0.379911000	-1.769238000
1	1.783839000	-0.985943000	-1.426268000
1	2.897817000	-0.414819000	-0.187456000

Ph_2S_2

16	-0.806978000	0.686853000	-1.723953000
16	0.806978000	-0.686853000	-1.723953000
6	-0.393188000	1.825574000	-0.399160000
6	-1.038835000	1.705072000	0.840537000
1	-1.755478000	0.898761000	0.996491000
6	0.528612000	2.863220000	-0.608959000
1	1.021589000	2.956567000	-1.576940000
6	0.806978000	3.765405000	0.419008000
1	1.523936000	4.571122000	0.251939000
6	-0.759567000	2.615740000	1.864036000
1	-1.264769000	2.518779000	2.826521000
6	0.163457000	3.644157000	1.656103000
1	0.380116000	4.354074000	2.455849000
6	0.393188000	-1.825574000	-0.399160000
6	-0.528612000	-2.863220000	-0.608959000
6	1.038835000	-1.705072000	0.840537000
6	-0.806978000	-3.765405000	0.419008000
6	0.759567000	-2.615740000	1.864036000
6	-0.163457000	-3.644157000	1.656103000
1	-1.021589000	-2.956567000	-1.576940000
1	1.755478000	-0.898761000	0.996491000
1	-1.523936000	-4.571122000	0.251939000
1	1.264769000	-2.518779000	2.826521000
1	-0.380116000	-4.354074000	2.455849000

Ph_2Se_2

34	-0.727755000	0.942261000	-1.365313000
34	0.727755000	-0.942261000	-1.365313000
6	0.021788000	2.019635000	0.060967000
6	-0.531160000	1.948897000	1.348248000
1	-1.355819000	1.264344000	1.547340000
6	1.081632000	2.901828000	-0.197091000
1	1.508393000	2.958054000	-1.198821000
6	1.586842000	3.702931000	0.829903000
1	2.411226000	4.388177000	0.624633000
6	-0.021788000	2.755258000	2.370937000
1	-0.455457000	2.697393000	3.370864000
6	1.036965000	3.630952000	2.114205000
1	1.432575000	4.259548000	2.913621000
6	-0.021788000	-2.019635000	0.060967000
6	-1.081632000	-2.901828000	-0.197091000
6	0.531160000	-1.948897000	1.348248000
6	-1.586842000	-3.702931000	0.829903000
6	0.021788000	-2.755258000	2.370937000
6	-1.036965000	-3.630952000	2.114205000
1	-1.508393000	-2.958054000	-1.198821000
1	1.355819000	-1.264344000	1.547340000
1	-2.411226000	-4.388177000	0.624633000

1	0.455457000	-2.697393000	3.370864000
1	-1.432575000	-4.259548000	2.913621000

Ph_2Te_2

52	-0.978743000	0.973672000	-1.168712000
52	0.978743000	-0.973672000	-1.168712000
6	-0.250169000	2.247027000	0.410156000
6	-0.697644000	2.054598000	1.726042000
1	-1.392631000	1.246247000	1.955902000
6	0.642403000	3.291410000	0.126115000
1	0.993964000	3.449662000	-0.894053000
6	1.086070000	4.131496000	1.152140000
1	1.780934000	4.941726000	0.923677000
6	-0.250169000	2.898426000	2.748045000
1	-0.602514000	2.742618000	3.769373000
6	0.641956000	3.936223000	2.463481000
1	0.989477000	4.593523000	3.262259000
6	0.250169000	-2.247027000	0.410156000
6	-0.642403000	-3.291410000	0.126115000
6	0.697644000	-2.054598000	1.726042000
6	-1.086070000	-4.131496000	1.152140000
6	0.250169000	-2.898426000	2.748045000
6	-0.641956000	-3.936223000	2.463481000
1	-0.993964000	-3.449662000	-0.894053000
1	1.392631000	-1.246247000	1.955902000
1	-1.780934000	-4.941726000	0.923677000
1	0.602514000	-2.742618000	3.769373000
1	-0.989477000	-4.593523000	3.262259000

PhS

16	2.308057000	0.000003000	-0.000053000
6	0.578722000	-0.000098000	-0.000099000
6	-0.149486000	1.221261000	0.000102000
6	-0.149630000	-1.221353000	0.000013000
6	-1.539695000	1.216046000	0.000143000
6	-1.539811000	-1.215966000	0.000247000
6	-2.239235000	0.000082000	-0.000423000
1	0.405338000	2.159542000	0.000374000
1	0.405076000	-2.159710000	0.000273000
1	-2.086928000	2.160103000	0.000390000
1	-2.087104000	-2.159990000	0.000439000
1	-3.330492000	0.000174000	-0.000536000

PhSe

34	1.849360000	0.000008000	0.000066000
6	-0.068859000	0.000512000	-0.000273000
6	-0.774297000	1.214463000	-0.000016000
6	-0.773596000	-1.214001000	0.000022000
6	-2.171587000	1.206494000	-0.000236000
6	-2.170825000	-1.206963000	-0.000279000
6	-2.876372000	-0.000418000	0.000601000
1	-0.240012000	2.165810000	-0.000546000
1	-0.238799000	-2.165068000	-0.000513000
1	-2.710266000	2.155879000	-0.000492000
1	-2.708874000	-2.156705000	-0.000512000
1	-3.967063000	-0.000692000	0.000894000

PhTe

52	0.000000000	1.582989000	0.000000000
6	0.000687000	-0.536708000	0.000000000

6	0.000085000	-1.251056000	-1.215626000
6	0.000085000	-1.251056000	1.215626000
6	-0.000253000	-2.646780000	-1.211577000
6	-0.000253000	-2.646780000	1.211577000
6	-0.000147000	-3.347331000	0.000000000
1	0.000233000	-0.709185000	-2.161777000
1	0.000233000	-0.709185000	2.161777000
1	-0.000515000	-3.190132000	-2.158156000
1	-0.000515000	-3.190132000	2.158156000
1	-0.000675000	-4.438619000	0.000000000

PhSH

16	2.294009000	-0.083877000	-0.000136000
6	0.509367000	-0.000593000	0.000250000
6	-0.194841000	1.212531000	0.000052000
6	-0.201001000	-1.211357000	0.000200000
6	-1.591754000	1.209938000	-0.000006000
6	-1.597181000	-1.202968000	0.000017000
6	-2.300433000	0.005265000	0.000112000
1	0.342752000	2.161891000	0.000433000
1	0.338236000	-2.160351000	0.000005000
1	-2.127237000	2.160909000	-0.000613000
1	-2.137066000	-2.151478000	-0.000609000
1	-3.391094000	0.007001000	-0.000918000
1	2.525319000	1.247168000	0.000117000

PhSeH

34	1.835756000	0.000000000	-0.044442000
6	-0.110180000	0.000000000	0.007659000
6	-0.811855000	1.212753000	0.001799000
6	-0.811855000	-1.212753000	0.001798000
6	-2.210322000	1.209418000	0.000905000
6	-2.210322000	-1.209418000	0.000904000
6	-2.910992000	0.000000000	0.002892000
1	-0.265232000	2.156056000	-0.002846000
1	-0.265232000	-2.156056000	-0.002849000
1	-2.751833000	2.157042000	-0.001765000
1	-2.751834000	-2.157042000	-0.001766000
1	-4.002164000	0.000000000	0.001480000
1	2.013746000	-0.000016000	1.423044000

PhTeH

52	1.577813000	0.000003000	-0.033200000
6	-0.579504000	0.000003000	0.008651000
6	-1.283150000	1.212402000	0.002638000
6	-1.283146000	-1.212400000	0.002623000
6	-2.682224000	1.209058000	0.000473000
6	-2.682220000	-1.209060000	0.000464000
6	-3.383161000	-0.000002000	0.001071000
1	-0.743433000	2.159854000	0.000823000
1	-0.743427000	-2.159850000	0.000789000
1	-3.223314000	2.157033000	-0.001901000
1	-3.223308000	-2.157037000	-0.001920000
1	-4.474416000	-0.000003000	-0.001273000
1	1.722086000	-0.000169000	1.634385000

PhSP{W(CO)$_5$}$_2$

74	-1.684585000	-1.292988000	0.017100000
74	2.611640000	0.302252000	-0.001551000
15	0.113853000	0.438468000	-0.035059000

16	-0.305474000	2.500839000	-0.138782000
8	0.421780000	-3.369349000	-1.261216000
8	-0.754840000	-2.124417000	3.004472000
8	2.421941000	-2.519181000	1.547949000
8	-3.719802000	-3.774238000	-0.003934000
8	5.803794000	-0.013636000	0.166204000
8	2.635930000	1.949297000	2.781335000
8	-2.742964000	-0.455520000	-2.919640000
8	3.044040000	3.087180000	-1.584864000
8	2.626901000	-1.221571000	-2.856657000
8	-4.109054000	0.356253000	1.374222000
6	-2.997412000	-2.881356000	0.007548000
6	-1.068795000	-1.831750000	1.942612000
6	-0.301463000	-2.602518000	-0.808418000
6	2.464846000	-1.513393000	0.996884000
6	2.612413000	-0.693998000	-1.839581000
6	4.662698000	0.101567000	0.101631000
6	-2.863828000	2.697361000	-1.221402000
1	-2.430800000	2.313634000	-2.144243000
6	-3.209116000	-0.152391000	0.878999000
6	-2.360292000	-0.746148000	-1.878080000
6	2.858400000	2.107725000	-1.018515000
6	-4.209276000	3.068723000	-1.174527000
1	-4.829551000	2.957552000	-2.064994000
6	2.628018000	1.356080000	1.800643000
6	-2.066690000	2.837045000	-0.076279000
6	-3.954057000	3.739054000	1.138295000
1	-4.377220000	4.144130000	2.058425000
6	-4.756059000	3.586964000	0.003358000
1	-5.807099000	3.876636000	0.035275000
6	-2.609326000	3.365284000	1.103902000
1	-1.979806000	3.484003000	1.985958000

PhSeP{W(CO)$_5$}$_2$

74	-2.643765000	0.272444000	0.010464000
74	1.592646000	-1.490039000	0.012786000
34	0.404737000	2.490060000	-0.144332000
15	-0.135385000	0.314997000	-0.023677000
8	2.752677000	-0.594816000	-2.867451000
8	-0.556394000	-3.434284000	-1.397711000
8	-2.619772000	1.772280000	2.875899000
8	-2.559099000	-2.627393000	1.418255000
8	-5.840391000	0.028050000	0.173926000
8	-3.053898000	3.132188000	-1.437069000
8	4.014879000	0.041532000	1.506678000
8	0.550089000	-2.397473000	2.939916000
8	-2.698118000	-1.106701000	-2.917513000
8	3.541488000	-4.038306000	-0.044209000
6	0.184894000	-2.715965000	-0.897227000
6	-2.558813000	-1.594692000	0.917976000
6	2.335777000	-0.904013000	-1.844470000
6	2.327211000	2.706533000	-0.052249000
6	3.123414000	-0.428628000	0.960988000
6	-2.627859000	1.231960000	1.865113000
6	2.849800000	-3.121410000	-0.019524000
6	-2.865992000	2.126682000	-0.917621000
6	2.893446000	3.184447000	1.137473000
1	2.269017000	3.347027000	2.016366000

6	3.124604000	2.506551000	-1.187293000
1	2.679441000	2.157720000	-2.118287000
6	-2.670910000	-0.630581000	-1.875761000
6	-4.696827000	0.119817000	0.111335000
6	4.495785000	2.767883000	-1.120560000
1	5.117256000	2.608798000	-2.003051000
6	0.903705000	-2.076614000	1.898817000
6	4.264140000	3.448502000	1.191420000
1	4.706131000	3.814182000	2.119308000
6	5.066309000	3.237155000	0.066291000
1	6.136858000	3.440933000	0.113507000

PhTeP{W(CO)$_5$}$_2$

74	2.695186000	-0.307131000	0.020707000
74	-1.426712000	1.734483000	0.006200000
52	-0.597122000	-2.515660000	-0.124417000
15	0.176966000	-0.188111000	-0.008821000
8	-2.760767000	0.782374000	-2.778396000
8	0.780082000	3.463210000	-1.588077000
8	2.600246000	-1.617930000	2.976304000
8	2.805549000	2.677537000	1.238234000
8	5.897341000	-0.210992000	0.166558000
8	3.010583000	-3.258300000	-1.250501000
8	-3.814688000	0.365082000	1.700094000
8	-0.204326000	2.726148000	2.834011000
8	2.796759000	0.881225000	-2.989200000
8	-3.236284000	4.381683000	-0.081661000
6	0.012755000	2.824699000	-1.023025000
6	2.728021000	1.616944000	0.807749000
6	-2.284329000	1.110674000	-1.787775000
6	-2.743796000	-2.516603000	-0.023012000
6	-2.948926000	0.788917000	1.080199000
6	2.633691000	-1.144265000	1.933022000
6	-2.593547000	3.429706000	-0.045999000
6	2.845663000	-2.218220000	-0.792136000
6	-3.366183000	-2.907630000	1.171129000
1	-2.772984000	-3.130453000	2.058868000
6	-3.515745000	-2.235946000	-1.159431000
1	-3.040602000	-1.947627000	-2.096829000
6	2.754434000	0.473229000	-1.919527000
6	4.750035000	-0.251931000	0.110663000
6	-4.909218000	-2.330154000	-1.091361000
1	-5.507315000	-2.106899000	-1.976167000
6	-0.619836000	2.372355000	1.826859000
6	-4.759307000	-3.004574000	1.228335000
1	-5.240837000	-3.302308000	2.160969000
6	-5.531464000	-2.712998000	0.100301000
1	-6.618862000	-2.786281000	0.149186000

Mes$_2$S$_2$

16	0.212198000	1.074476000	0.000229000
16	-0.212198000	-1.074476000	0.000229000
6	1.999868000	1.015430000	0.001822000
6	4.817402000	1.030674000	0.003807000
6	2.697556000	1.017292000	1.231716000
6	2.700793000	1.010814000	-1.229684000
6	4.098634000	1.020928000	-1.199438000
1	4.644435000	1.019554000	-2.145395000
6	4.098634000	1.027722000	1.203423000

1	4.642570000	1.031664000	2.150032000
6	6.325662000	1.042852000	-0.007274000
1	6.723483000	0.164150000	-0.537784000
1	6.737947000	1.040434000	1.009527000
1	6.709505000	1.933877000	-0.527505000
6	1.983119000	0.991014000	-2.556013000
1	1.328127000	0.112103000	-2.637417000
1	2.701772000	0.967154000	-3.384302000
1	1.341542000	1.875359000	-2.675364000
6	1.980271000	1.004250000	2.558261000
1	1.338883000	1.889235000	2.673808000
1	2.699102000	0.984355000	3.386536000
1	1.325386000	0.125722000	2.644484000
6	-1.999868000	-1.015430000	0.001822000
6	-2.697556000	-1.017292000	1.231716000
6	-2.700793000	-1.010814000	-1.229684000
6	-4.098634000	-1.027722000	1.203423000
6	-4.098634000	-1.020928000	-1.199438000
6	-4.817402000	-1.030674000	0.003807000
1	-4.642570000	-1.031664000	2.150032000
1	-4.644435000	-1.019554000	-2.145395000
6	-1.980271000	-1.004250000	2.558261000
1	-1.338883000	-1.889235000	2.673808000
1	-1.325386000	-0.125722000	2.644484000
1	-2.699102000	-0.984355000	3.386536000
6	-6.325662000	-1.042852000	-0.007274000
1	-6.737947000	-1.040434000	1.009527000
1	-6.723483000	-0.164150000	-0.537784000
1	-6.709505000	-1.933877000	-0.527505000
6	-1.983119000	-0.991014000	-2.556013000
1	-2.701772000	-0.967154000	-3.384302000
1	-1.328127000	-0.112103000	-2.637417000
1	-1.341542000	-1.875359000	-2.675364000

Mes_2Se_2

34	-0.972909000	0.740055000	-0.088262000
34	0.972909000	-0.740055000	-0.088262000
6	0.001835000	2.412526000	-0.008713000
6	1.327748000	4.896299000	0.103549000
6	0.314877000	2.979702000	1.247330000
6	0.355588000	3.070668000	-1.211867000
6	1.010999000	4.303975000	-1.126059000
1	1.286053000	4.817049000	-2.050096000
6	0.972909000	4.217866000	1.273231000
1	1.216616000	4.661539000	2.240562000
6	2.035577000	6.227533000	0.151583000
1	3.012316000	6.173747000	-0.353435000
1	2.205850000	6.558188000	1.183866000
1	1.449949000	7.005228000	-0.362204000
6	0.056993000	2.488637000	-2.572222000
1	0.483145000	1.480912000	-2.675305000
1	0.471692000	3.125490000	-3.363441000
1	-1.025355000	2.390849000	-2.737552000
6	-0.026906000	2.302034000	2.551494000
1	-1.113703000	2.188764000	2.670980000
1	0.355985000	2.882404000	3.400069000
1	0.403037000	1.291716000	2.597520000
6	-0.001835000	-2.412526000	-0.008713000

6	-0.314877000	-2.979702000	1.247330000
6	-0.355588000	-3.070668000	-1.211867000
6	-0.972909000	-4.217866000	1.273231000
6	-1.010999000	-4.303975000	-1.126059000
6	-1.327748000	-4.896299000	0.103549000
1	-1.216616000	-4.661539000	2.240562000
1	-1.286053000	-4.817049000	-2.050096000
6	0.026906000	-2.302034000	2.551494000
1	1.113703000	-2.188764000	2.670980000
1	-0.403037000	-1.291716000	2.597520000
1	-0.355985000	-2.882404000	3.400069000
6	-2.035577000	-6.227533000	0.151583000
1	-2.205850000	-6.558188000	1.183866000
1	-3.012316000	-6.173747000	-0.353435000
1	-1.449949000	-7.005228000	-0.362204000
6	-0.056993000	-2.488637000	-2.572222000
1	-0.471692000	-3.125490000	-3.363441000
1	-0.483145000	-1.480912000	-2.675305000
1	1.025355000	-2.390849000	-2.737552000

Mes_2Te_2

52	-1.100419000	0.881831000	-0.452938000
52	1.100419000	-0.881831000	-0.452938000
6	0.001626000	2.679616000	0.042900000
6	1.353488000	5.078761000	0.668110000
6	0.346728000	2.960121000	1.384163000
6	0.330562000	3.589446000	-0.992112000
6	0.999054000	4.772274000	-0.651264000
1	1.253923000	5.476546000	-1.446272000
6	1.019140000	4.159710000	1.665432000
1	1.287075000	4.377910000	2.701164000
6	2.074636000	6.363895000	0.990379000
1	3.033225000	6.424671000	0.452526000
1	2.282798000	6.452331000	2.064094000
1	1.479026000	7.238538000	0.686785000
6	-0.001626000	3.348606000	-2.446828000
1	0.403759000	2.389980000	-2.799210000
1	0.410295000	4.150740000	-3.072002000
1	-1.087488000	3.309201000	-2.614639000
6	0.038060000	2.024011000	2.525549000
1	-1.036335000	1.800862000	2.583064000
1	0.354718000	2.460385000	3.480874000
1	0.557438000	1.063379000	2.398429000
6	-0.001626000	-2.679616000	0.042900000
6	-0.346728000	-2.960121000	1.384163000
6	-0.330562000	-3.589446000	-0.992112000
6	-1.019140000	-4.159710000	1.665432000
6	-0.999054000	-4.772274000	-0.651264000
6	-1.353488000	-5.078761000	0.668110000
1	-1.287075000	-4.377910000	2.701164000
1	-1.253923000	-5.476546000	-1.446272000
6	-0.038060000	-2.024011000	2.525549000
1	1.036335000	-1.800862000	2.583064000
1	-0.557438000	-1.063379000	2.398429000
1	-0.354718000	-2.460385000	3.480874000
6	-2.074636000	-6.363895000	0.990379000
1	-2.282798000	-6.452331000	2.064094000
1	-3.033225000	-6.424671000	0.452526000

1	-1.479026000	-7.238538000	0.686785000
6	0.001626000	-3.348606000	-2.446828000
1	-0.410295000	-4.150740000	-3.072002000
1	-0.403759000	-2.389980000	-2.799210000
1	1.087488000	-3.309201000	-2.614639000

MesS

16	-2.566098000	-0.009645000	0.000094000
6	-0.845372000	-0.001525000	-0.000037000
6	-0.122390000	1.242316000	-0.000036000
6	-0.109505000	-1.240561000	-0.000056000
6	1.270772000	1.215292000	0.000056000
6	1.279842000	-1.199925000	0.000048000
6	1.994647000	0.012667000	0.000099000
1	1.817356000	2.160221000	0.000142000
1	1.836196000	-2.139586000	0.000087000
6	-0.840379000	2.564672000	-0.000105000
1	-1.493940000	2.660348000	-0.878803000
1	-1.494193000	2.660358000	0.878396000
1	-0.124017000	3.395487000	-0.000028000
6	3.499387000	0.005294000	0.000016000
1	3.912499000	1.021353000	0.002164000
1	3.888814000	-0.525485000	0.882829000
1	3.888642000	-0.521544000	-0.885263000
6	-0.817000000	-2.568871000	-0.000102000
1	-0.093899000	-3.393817000	-0.000376000
1	-1.469760000	-2.669727000	0.878606000
1	-1.470138000	-2.669445000	-0.878555000

MesSe

34	-2.208049000	-0.003295000	0.000039000
6	-0.283790000	0.001549000	-0.000010000
6	0.404609000	1.230088000	-0.000068000
6	0.411149000	-1.226722000	-0.000090000
6	1.805950000	1.203627000	-0.000132000
6	1.809198000	-1.194467000	-0.000192000
6	2.530569000	0.007416000	-0.000245000
1	2.344093000	2.154325000	-0.000236000
1	2.351700000	-2.143045000	-0.000307000
6	-0.340660000	2.539960000	0.000010000
1	-0.988816000	2.630205000	-0.887214000
1	-0.989652000	2.629617000	0.886676000
1	0.349624000	3.392685000	0.000654000
6	4.039864000	-0.001172000	0.000246000
1	4.448184000	1.017548000	-0.005486000
1	4.435063000	-0.517512000	0.888782000
1	4.435688000	-0.527932000	-0.881805000
6	-0.329997000	-2.539088000	0.000036000
1	0.363094000	-3.389486000	-0.000626000
1	-0.977747000	-2.630958000	0.887341000
1	-0.978935000	-2.630555000	-0.886443000

MesTe

52	-2.000477000	-0.002264000	-0.000096000
6	0.125745000	0.001931000	0.000117000
6	2.957982000	0.007676000	-0.000105000
6	0.835531000	1.235316000	0.000127000
6	0.841702000	-1.231106000	0.000087000
6	2.238250000	-1.196051000	-0.000019000
1	2.787353000	-2.140119000	-0.000019000

6	2.235574000	1.205820000	-0.000014000
1	2.780474000	2.151898000	-0.000008000
6	4.464583000	-0.002352000	-0.000221000
1	4.854802000	-0.528890000	0.884504000
1	4.877361000	1.014114000	-0.000652000
1	4.854603000	-0.529578000	-0.884622000
6	0.158886000	-2.577526000	0.000302000
1	-0.487386000	-2.700194000	0.880661000
1	0.901426000	-3.385359000	-0.000063000
1	-0.488301000	-2.700099000	-0.879368000
6	0.149763000	2.580133000	0.000305000
1	-0.496643000	2.701958000	-0.880031000
1	0.890467000	3.389677000	0.000963000
1	-0.497456000	2.701264000	0.880139000

MesSH

16	-2.569373000	0.069146000	0.000063000
6	-0.776412000	-0.015233000	0.000035000
6	-0.096002000	1.220776000	-0.000020000
6	-0.060586000	-1.233872000	0.000021000
6	1.304712000	1.215585000	-0.000084000
6	1.338249000	-1.177912000	-0.000076000
6	2.045870000	0.030510000	-0.000122000
1	1.828477000	2.173934000	-0.000203000
1	1.894338000	-2.118261000	-0.000109000
6	-0.850653000	2.526289000	0.000015000
1	-1.501804000	2.614606000	-0.884401000
1	-1.501597000	2.614660000	0.884575000
1	-0.160515000	3.378452000	-0.000096000
6	3.555215000	0.040772000	0.000087000
1	3.950257000	1.064736000	-0.003146000
1	3.957381000	-0.472602000	0.887234000
1	3.957713000	-0.478435000	-0.883472000
6	-0.746123000	-2.577209000	0.000040000
1	-0.008443000	-3.388455000	0.000190000
1	-1.384997000	-2.709809000	0.888307000
1	-1.384794000	-2.709937000	-0.888359000
1	-2.821669000	-1.253447000	-0.000886000

MesSeH

34	-0.332943000	2.177651000	0.000000000
6	0.000000000	0.266241000	0.000000000
6	-1.144838000	-0.557251000	0.000000000
6	1.296058000	-0.295682000	0.000000000
6	-0.971635000	-1.947894000	0.000000000
6	1.408198000	-1.691989000	0.000000000
6	0.294036000	-2.539969000	0.000000000
1	-1.859746000	-2.583540000	0.000000000
1	2.408525000	-2.130982000	0.000000000
6	-2.535507000	0.026556000	0.000000000
1	-2.706722000	0.659279000	0.885915000
1	-2.706722000	0.659279000	-0.885915000
1	-3.294492000	-0.764835000	0.000000000
6	0.466440000	-4.039397000	0.000000000
1	-0.502056000	-4.555695000	0.000000000
1	1.027853000	-4.375824000	-0.885334000
1	1.027853000	-4.375824000	0.885334000
6	2.552495000	0.538485000	0.000000000
1	3.442223000	-0.102505000	0.000000000

1	2.608900000	1.188274000	-0.887666000
1	2.608900000	1.188274000	0.887666000
1	1.074083000	2.599377000	0.000000000

MesTeH

52	-1.990096000	0.027794000	0.000016000
6	0.169661000	-0.045820000	-0.000015000
6	0.824219000	1.202924000	-0.000017000
6	0.909059000	-1.248994000	0.000006000
6	2.226365000	1.228891000	-0.000019000
6	2.308058000	-1.162837000	-0.000010000
6	2.990597000	0.059520000	-0.000032000
1	2.730821000	2.197636000	-0.000019000
1	2.884284000	-2.091038000	0.000008000
6	0.059416000	2.503442000	0.000003000
1	-0.587802000	2.591019000	-0.888108000
1	-0.587818000	2.590996000	0.888105000
1	0.740417000	3.363014000	0.000033000
6	4.499194000	0.100011000	0.000004000
1	4.874296000	1.131415000	-0.000375000
1	4.910768000	-0.408566000	0.885489000
1	4.910834000	-0.409257000	-0.885049000
6	0.268501000	-2.614448000	0.000056000
1	1.032892000	-3.400862000	0.000221000
1	-0.367263000	-2.762616000	0.886445000
1	-0.367040000	-2.762787000	-0.886467000
1	-2.219818000	-1.620364000	-0.000964000

MesSP{W(CO)$_5$}$_2$

74	2.754850000	-0.648601000	-0.000189000
74	-1.145917000	1.769384000	-0.000317000
16	-0.531493000	-2.232441000	0.001840000
15	0.276404000	-0.289791000	0.000757000
8	-2.599509000	4.627580000	-0.003248000
8	5.946352000	-1.011004000	-0.001484000
8	1.531928000	3.552067000	-0.005361000
8	2.503759000	-2.950858000	-2.254150000
8	3.084401000	1.585806000	2.310159000
8	-4.182475000	0.675431000	0.003334000
8	3.082120000	1.579878000	-2.316598000
8	-1.202200000	1.742926000	3.235341000
8	2.505859000	-2.945161000	2.259819000
8	-1.208072000	1.733722000	-3.235739000
6	2.585873000	-2.130848000	-1.456969000
6	0.609507000	2.868839000	-0.003537000
6	-2.325214000	-2.240036000	0.003345000
6	4.804758000	-0.881268000	-0.000984000
6	-2.088299000	3.598665000	-0.002141000
6	2.955513000	0.803106000	1.481958000
6	-5.116951000	-2.528984000	0.005440000
6	-3.009151000	-2.317607000	1.236274000
6	-3.011918000	-2.322360000	-1.231098000
6	2.587300000	-2.127165000	1.460504000
6	-3.067506000	0.943757000	0.002445000
6	2.954036000	0.799323000	-1.486252000
6	-4.401507000	-2.462986000	-1.198058000
1	-4.944113000	-2.525208000	-2.143439000
6	-4.402026000	-2.457750000	1.205269000
1	-4.942990000	-2.515121000	2.151492000

6	-6.617348000	-2.673050000	-0.006111000
1	-7.087819000	-1.815022000	-0.509714000
1	-7.026514000	-2.735525000	1.009660000
1	-6.923069000	-3.577072000	-0.554103000
6	-1.176822000	1.749353000	-2.089976000
6	-1.172962000	1.755287000	2.089496000
6	-2.293789000	-2.270431000	-2.556698000
1	-1.792783000	-1.303300000	-2.707038000
1	-2.998181000	-2.417201000	-3.383598000
1	-1.514670000	-3.043074000	-2.624439000
6	-2.291806000	-2.261147000	2.562014000
1	-1.508432000	-3.029329000	2.630590000
1	-2.995577000	-2.411434000	3.388826000
1	-1.796455000	-1.291058000	2.712299000

MesSeP{W(CO)$_5$}$_2$

74	2.800527000	-0.632135000	-0.000473000
74	-1.024424000	1.910858000	-0.000284000
34	-0.604449000	-2.239098000	0.003823000
15	0.325632000	-0.201271000	0.001050000
8	-2.368301000	4.820790000	-0.002328000
8	5.984282000	-1.040996000	-0.003575000
8	1.708326000	3.608073000	-0.001750000
8	2.526269000	-2.921021000	-2.264590000
8	3.175834000	1.589912000	2.315757000
8	-4.104077000	0.946471000	-0.000751000
8	3.172083000	1.587992000	-2.319096000
8	-1.084617000	1.867263000	3.235250000
8	2.530713000	-2.919037000	2.266206000
8	-1.084514000	1.863390000	-3.235777000
6	2.613822000	-2.106200000	-1.462267000
6	0.766127000	2.952254000	-0.001095000
6	-2.538993000	-2.106949000	0.003686000
6	4.844213000	-0.896370000	-0.002373000
6	-1.897142000	3.772634000	-0.001552000
6	3.029433000	0.812925000	1.485304000
6	-5.344748000	-2.181635000	0.003509000
6	-3.227111000	-2.128830000	1.235530000
6	-3.228231000	-2.135122000	-1.230777000
6	2.616611000	-2.104939000	1.462971000
6	-2.978098000	1.164274000	-0.000133000
6	3.026982000	0.811670000	-1.487784000
6	-4.625391000	-2.169784000	-1.199021000
1	-5.170416000	-2.188125000	-2.144876000
6	-4.627500000	-2.162885000	1.203533000
1	-5.172184000	-2.175282000	2.149293000
6	-6.851857000	-2.211368000	-0.009114000
1	-7.255675000	-1.319625000	-0.512015000
1	-7.265267000	-2.243711000	1.006371000
1	-7.224906000	-3.089051000	-0.558202000
6	-1.053576000	1.885401000	-2.090100000
6	-1.053631000	1.887986000	2.089549000
6	-2.515328000	-2.128822000	-2.561361000
1	-1.918851000	-1.215137000	-2.695246000
1	-3.235805000	-2.186263000	-3.385601000
1	-1.820580000	-2.976084000	-2.653368000
6	-2.516800000	-2.116232000	2.567370000
1	-1.819103000	-2.960592000	2.663241000

1	-3.238541000	-2.174140000	3.390491000
1	-1.924193000	-1.199868000	2.700164000

MesTeP{W(CO)$_5$}$_2$

74	-2.857325000	-0.668819000	0.032305000
74	0.826299000	2.086314000	-0.001125000
52	0.756377000	-2.267904000	-0.202522000
15	-0.395048000	-0.112256000	-0.036375000
8	2.020341000	5.058437000	-0.053847000
8	-1.944497000	3.586447000	-0.660435000
8	-3.305480000	1.848914000	2.004270000
8	-6.017124000	-1.172842000	0.238654000
8	3.875578000	1.270605000	0.674129000
8	-2.399269000	-2.622484000	2.564330000
8	1.481422000	1.768857000	-3.150904000
8	-2.648954000	-3.226824000	-1.928088000
8	-3.356840000	1.175478000	-2.578788000
6	-0.984044000	3.003521000	-0.425547000
8	0.271538000	2.353987000	3.178031000
6	3.655589000	-1.788206000	-1.207904000
6	3.484692000	-1.987603000	1.241339000
6	2.881707000	-1.934739000	-0.036981000
6	1.601646000	3.987902000	-0.032093000
6	-4.883670000	-0.996252000	0.161427000
6	1.242675000	1.882806000	-2.034801000
6	5.676654000	-1.714311000	0.178258000
6	-3.124762000	0.963989000	1.297398000
6	5.046802000	-1.675084000	-1.068657000
1	5.654327000	-1.556327000	-1.967765000
6	-2.559315000	-1.922191000	1.670084000
6	2.768850000	1.448957000	0.432291000
6	3.057841000	-1.752900000	-2.594760000
1	2.483701000	-2.665199000	-2.813094000
1	3.845203000	-1.661493000	-3.352366000
1	2.370390000	-0.905345000	-2.720826000
6	0.456988000	2.259812000	2.051223000
6	4.876816000	-1.874849000	1.316948000
1	5.352211000	-1.907874000	2.299345000
6	-3.170099000	0.537887000	-1.645015000
6	2.695529000	-2.147753000	2.519547000
1	1.978487000	-1.325739000	2.657350000
1	3.365147000	-2.161293000	3.387669000
1	2.113804000	-3.081212000	2.526133000
6	-2.694868000	-2.317230000	-1.229198000
6	7.173212000	-1.587129000	0.307139000
1	7.656429000	-1.476715000	-0.671435000
1	7.603189000	-2.470900000	0.802433000
1	7.440003000	-0.712126000	0.918962000

Cp*P{W(CO)$_5$}$_2$·SHPh

16	0.210895000	1.918311000	1.409102000
15	-0.128548000	0.401365000	-0.402783000
74	-2.562710000	-0.505106000	0.465790000
74	1.732394000	-1.520606000	-0.646159000

6	-0.034543000	1.893325000	-1.760914000
6	2.775151000	-3.243440000	-0.795692000
6	2.644114000	-0.969415000	-2.416023000
6	1.056411000	-2.247906000	1.182939000
6	0.276561000	-2.446638000	-1.809514000
6	3.391125000	-0.737133000	0.323483000
6	-4.333664000	-1.148987000	1.178009000
6	-3.332539000	-0.677573000	-1.462323000
6	-1.841083000	-0.505784000	2.398273000
6	-3.280004000	1.410375000	0.798220000
6	-2.077802000	-2.522436000	0.351989000
6	-1.162777000	2.904675000	-1.598994000
6	-0.639691000	4.113972000	-1.260938000
6	0.832976000	4.015453000	-1.237374000
6	1.212096000	2.741702000	-1.563269000
6	-0.097574000	1.190037000	-3.129122000
6	-2.568333000	2.658250000	-2.045872000
6	-1.367289000	5.407787000	-1.049048000
6	1.709127000	5.207343000	-0.982798000
6	2.608575000	2.263743000	-1.787547000
8	-3.792291000	-0.840623000	-2.503409000
8	-5.354997000	-1.498966000	1.587860000
8	-1.930758000	-3.661905000	0.361242000
8	-3.745072000	2.428738000	1.067158000
8	-1.466230000	-0.527618000	3.488302000
8	3.355785000	-4.237341000	-0.873927000
8	0.783611000	-2.700935000	2.202869000
8	-0.449224000	-2.987097000	-2.516173000
8	4.388859000	-0.405014000	0.791039000
8	3.223055000	-0.750719000	-3.387855000
1	-1.015021000	0.598207000	-3.236314000
1	0.755286000	0.525906000	-3.289895000
1	-0.092945000	1.949736000	-3.923559000
1	-2.917823000	1.653355000	-1.805427000
1	-2.638850000	2.764585000	-3.141056000
1	-3.269981000	3.374149000	-1.604424000
1	-1.068475000	5.886314000	-0.103583000
1	-2.453125000	5.269838000	-1.022714000
1	-1.140399000	6.129058000	-1.850986000
1	1.496892000	5.661033000	-0.001959000
1	1.524290000	5.993423000	-1.730145000
1	2.775804000	4.961781000	-1.018311000
1	2.877307000	1.436403000	-1.119511000
1	3.336468000	3.068841000	-1.639515000
1	2.740917000	1.892468000	-2.813728000
1	0.619979000	2.917411000	0.553738000
6	1.788711000	1.708970000	2.239349000
6	1.861347000	0.775051000	3.280570000
6	2.885368000	2.520707000	1.921594000

6	3.051427000	0.650111000	3.999620000
6	4.064059000	2.391646000	2.656261000
6	4.150968000	1.454978000	3.690192000
1	0.998300000	0.162068000	3.536999000
1	2.818797000	3.249143000	1.114903000
1	3.113621000	-0.079087000	4.807598000
1	4.920076000	3.021528000	2.412976000
1	5.077947000	1.352059000	4.255085000

Cp*P{W(CO)$_5$}$_2$·SeHPh

74	-1.952273000	0.925033000	-0.958416000
6	-0.850187000	-1.869775000	1.659566000
6	-3.276466000	1.395775000	-2.400678000
6	-3.559041000	0.669918000	0.344419000
6	-0.438769000	1.395360000	-2.299603000
6	-2.224932000	-0.972227000	-1.816277000
6	-2.091466000	2.958990000	-0.523306000
6	-1.999332000	-1.387655000	2.533126000
6	-3.141124000	-2.007780000	2.133306000
6	-2.856703000	-2.903161000	1.001206000
6	-1.526342000	-2.868208000	0.718635000
6	0.257436000	-2.504207000	2.517426000
6	-1.861381000	-0.599924000	3.810625000
6	-4.484026000	-1.926947000	2.793275000
6	-3.921756000	-3.731796000	0.349022000
6	-0.796107000	-3.728653000	-0.264098000
8	-4.031409000	1.622067000	-3.242865000
8	0.329954000	1.722640000	-3.084446000
8	-2.470079000	-1.917361000	-2.413406000
8	-2.270174000	4.085413000	-0.389304000
8	-4.520778000	0.674571000	0.970600000
1	0.741238000	-1.764411000	3.167380000
1	1.032587000	-2.970435000	1.904674000
1	-0.186722000	-3.281909000	3.154945000
1	-2.296519000	-1.159830000	4.651893000
1	-2.382956000	0.367894000	3.772350000
1	-0.818004000	-0.391128000	4.065120000
1	-5.285268000	-1.768105000	2.057747000
1	-4.536235000	-1.110980000	3.522197000
1	-4.719057000	-2.866545000	3.319358000
1	-4.705957000	-3.093559000	-0.087951000
1	-4.422680000	-4.382051000	1.083201000
1	-3.528325000	-4.367371000	-0.450588000
1	-0.207129000	-3.150935000	-0.988393000
1	-1.492347000	-4.350115000	-0.836899000
1	-0.091560000	-4.405360000	0.241687000
74	2.411988000	-1.005165000	-0.492702000
6	4.242350000	-1.286442000	-1.285287000
6	3.268146000	-0.834684000	1.385187000
6	1.566142000	-1.329863000	-2.362458000
6	2.760856000	0.996643000	-0.950501000
6	2.446205000	-3.051233000	-0.211509000
8	5.293780000	-1.437010000	-1.737580000

8	3.090865000	2.045020000	-1.282946000
8	3.776087000	-0.806847000	2.418116000
8	2.598733000	-4.187506000	-0.102653000
8	1.126264000	-1.555459000	-3.400016000
15	-0.064832000	-0.497997000	0.477840000
34	-0.311305000	1.440076000	1.788735000
6	1.257090000	2.562964000	1.613655000
6	1.199228000	3.741491000	0.858324000
6	2.393599000	2.269997000	2.380586000
6	2.290898000	4.612906000	0.855206000
6	3.481100000	3.145736000	2.366810000
6	3.433122000	4.315375000	1.602362000
1	0.312981000	3.987801000	0.278782000
1	2.429447000	1.370775000	2.991915000
1	2.246235000	5.525544000	0.259925000
1	4.365743000	2.911795000	2.960551000
1	4.285260000	4.996160000	1.592107000

Cp*P{W(CO)$_5$}$_2$·TeHPh

52	0.291815000	2.112856000	1.232046000
15	-0.166935000	0.246070000	-0.578623000
74	-2.615419000	-0.543022000	0.512741000
74	1.622738000	-1.788867000	-0.706210000
6	-0.106433000	1.563049000	-2.104401000
6	2.621130000	-3.538627000	-0.700851000
6	2.421285000	-1.505379000	-2.590633000
6	1.034281000	-2.281903000	1.226092000
6	0.076783000	-2.792066000	-1.671662000
6	3.342027000	-0.911177000	0.050142000
6	-4.352371000	-1.104449000	1.350232000
6	-3.468022000	-0.840858000	-1.367639000
6	-1.804454000	-0.409229000	2.399898000
6	-3.322195000	1.388081000	0.729852000
6	-2.167526000	-2.575582000	0.550775000
6	-1.154295000	2.661678000	-1.963708000
6	-0.532219000	3.870851000	-1.884123000
6	0.921295000	3.679237000	-2.016615000
6	1.196046000	2.346937000	-2.163178000
6	-0.349631000	0.707153000	-3.363642000
6	-2.614910000	2.451708000	-2.207407000
6	-1.168815000	5.226357000	-1.802484000
6	1.877974000	4.834952000	-2.064736000
6	2.538194000	1.752660000	-2.432493000
8	-3.971643000	-1.061641000	-2.376649000
8	-5.357761000	-1.409485000	1.830927000
8	-2.049470000	-3.712146000	0.665089000
8	-3.786297000	2.421439000	0.943452000
8	-1.377658000	-0.350590000	3.471216000
8	3.181591000	-4.547975000	-0.686809000
8	0.799383000	-2.615964000	2.300684000
8	-0.701934000	-3.378038000	-2.279285000
8	4.364390000	-0.515787000	0.401684000
8	2.926706000	-1.446926000	-3.624382000
1	-1.309813000	0.179668000	-3.313831000

1	0.439419000	-0.036163000	-3.509281000
1	-0.368805000	1.362333000	-4.246312000
1	-2.970032000	1.494250000	-1.824201000
1	-2.819657000	2.455448000	-3.291039000
1	-3.226036000	3.242814000	-1.758975000
1	-0.726452000	5.831526000	-0.996143000
1	-2.247090000	5.165749000	-1.621415000
1	-1.017978000	5.792547000	-2.736052000
1	1.776240000	5.478773000	-1.177297000
1	1.670438000	5.476748000	-2.935172000
1	2.922714000	4.514075000	-2.130081000
1	2.827640000	1.023347000	-1.665794000
1	3.314832000	2.524014000	-2.475142000
1	2.555472000	1.219384000	-3.393789000
1	1.100403000	3.044917000	0.080529000
6	2.124870000	1.634463000	2.240749000
6	2.093443000	0.702783000	3.285845000
6	3.306840000	2.314313000	1.920042000
6	3.263474000	0.446344000	4.006728000
6	4.466822000	2.052020000	2.652541000
6	4.447280000	1.118559000	3.692562000
1	1.175302000	0.176441000	3.546188000
1	3.336457000	3.036844000	1.104568000
1	3.243203000	-0.283290000	4.816861000
1	5.390587000	2.574040000	2.400259000
1	5.357457000	0.912359000	4.257017000

Cp*P{W(CO)$_5$}$_2$·SPh

74	-1.992750000	1.005900000	-0.807302000
6	-0.751392000	-1.954454000	1.588454000
6	-3.336923000	1.514408000	-2.212286000
6	-3.582615000	0.566188000	0.467793000
6	-0.506190000	1.658050000	-2.101454000
6	-2.173835000	-0.830207000	-1.808053000
6	-2.248005000	2.992674000	-0.219931000
6	-1.895187000	-1.566812000	2.513194000
6	-3.023616000	-2.201197000	2.098306000
6	-2.734852000	-3.011664000	0.904050000
6	-1.413430000	-2.911818000	0.597174000
6	0.394548000	-2.605744000	2.381972000
6	-1.752423000	-0.841643000	3.825755000
6	-4.353406000	-2.208027000	2.788966000
6	-3.786347000	-3.830462000	0.218145000
6	-0.674190000	-3.675414000	-0.456433000
8	-4.103666000	1.767030000	-3.036654000
8	0.243786000	2.087417000	-2.854549000
8	-2.375209000	-1.740713000	-2.471522000
8	-2.493920000	4.092226000	-0.000251000
8	-4.542301000	0.470030000	1.088945000
1	0.863730000	-1.895777000	3.074564000
1	1.174446000	-2.999313000	1.725498000
1	-0.009955000	-3.441203000	2.970889000
1	-2.130766000	-1.464066000	4.650482000
1	-2.318279000	0.100972000	3.850453000

1	-0.712345000	-0.591789000	4.055414000
1	-5.176070000	-2.030815000	2.081824000
1	-4.415051000	-1.441840000	3.569492000
1	-4.545306000	-3.186178000	3.259306000
1	-4.598490000	-3.191070000	-0.162481000
1	-4.252350000	-4.542918000	0.916784000
1	-3.388591000	-4.399978000	-0.627918000
1	-0.120736000	-3.027935000	-1.149579000
1	-1.359959000	-4.280113000	-1.059156000
1	0.064095000	-4.359755000	-0.012534000
74	2.443382000	-0.789125000	-0.528450000
6	4.263095000	-0.929461000	-1.381903000
6	3.357387000	-0.764317000	1.330883000
6	1.578754000	-0.972476000	-2.408731000
6	2.708466000	1.261331000	-0.781472000
6	2.545815000	-2.850481000	-0.431949000
8	5.307021000	-0.999546000	-1.869261000
8	2.988582000	2.353711000	-0.996986000
8	3.912533000	-0.817845000	2.337877000
8	2.733122000	-3.986514000	-0.422318000
8	1.135474000	-1.120098000	-3.458699000
15	-0.036209000	-0.479079000	0.501830000
16	-0.416212000	1.252478000	1.809262000
6	1.010226000	2.337385000	1.914279000
6	0.973404000	3.610777000	1.329738000
6	2.099283000	1.962583000	2.715199000
6	2.034985000	4.495006000	1.531189000
6	3.158284000	2.850690000	2.905600000
6	3.130290000	4.116279000	2.311224000
1	0.122007000	3.915721000	0.726590000
1	2.112350000	0.987341000	3.197040000
1	2.005592000	5.481729000	1.068096000
1	4.004821000	2.551594000	3.524631000
1	3.960502000	4.807839000	2.459678000

Cp*P{W(CO)$_5$}$_2$·SePh

74	-1.952273000	0.925033000	-0.958416000
6	-0.850187000	-1.869775000	1.659566000
6	-3.276466000	1.395775000	-2.400678000
6	-3.559041000	0.669918000	0.344419000
6	-0.438769000	1.395360000	-2.299603000
6	-2.224932000	-0.972227000	-1.816277000
6	-2.091466000	2.958990000	-0.523306000
6	-1.999332000	-1.387655000	2.533126000
6	-3.141124000	-2.007780000	2.133306000
6	-2.856703000	-2.903161000	1.001206000
6	-1.526342000	-2.868208000	0.718635000
6	0.257436000	-2.504207000	2.517426000
6	-1.861381000	-0.599924000	3.810625000
6	-4.484026000	-1.926947000	2.793275000
6	-3.921756000	-3.731796000	0.349022000
6	-0.796107000	-3.728653000	-0.264098000
8	-4.031409000	1.622067000	-3.242865000
8	0.329954000	1.722640000	-3.084446000

8	-2.470079000	-1.917361000	-2.413406000
8	-2.270174000	4.085413000	-0.389304000
8	-4.520778000	0.674571000	0.970600000
1	0.741238000	-1.764411000	3.167380000
1	1.032587000	-2.970435000	1.904674000
1	-0.186722000	-3.281909000	3.154945000
1	-2.296519000	-1.159830000	4.651893000
1	-2.382956000	0.367894000	3.772350000
1	-0.818004000	-0.391128000	4.065120000
1	-5.285268000	-1.768105000	2.057747000
1	-4.536235000	-1.110980000	3.522197000
1	-4.719057000	-2.866545000	3.319358000
1	-4.705957000	-3.093559000	-0.087951000
1	-4.422680000	-4.382051000	1.083201000
1	-3.528325000	-4.367371000	-0.450588000
1	-0.207129000	-3.150935000	-0.988393000
1	-1.492347000	-4.350115000	-0.836899000
1	-0.091560000	-4.405360000	0.241687000
74	2.411988000	-1.005165000	-0.492702000
6	4.242350000	-1.286442000	-1.285287000
6	3.268146000	-0.834684000	1.385187000
6	1.566142000	-1.329863000	-2.362458000
6	2.760856000	0.996643000	-0.950501000
6	2.446205000	-3.051233000	-0.211509000
8	5.293780000	-1.437010000	-1.737580000
8	3.090865000	2.045020000	-1.282946000
8	3.776087000	-0.806847000	2.418116000
8	2.598733000	-4.187506000	-0.102653000
8	1.126264000	-1.555459000	-3.400016000
15	-0.064832000	-0.497997000	0.477840000
34	-0.311305000	1.440076000	1.788735000
6	1.257090000	2.562964000	1.613655000
6	1.199228000	3.741491000	0.858324000
6	2.393599000	2.269997000	2.380586000
6	2.290898000	4.612906000	0.855206000
6	3.481100000	3.145736000	2.366810000
6	3.433122000	4.315375000	1.602362000
1	0.312981000	3.987801000	0.278782000
1	2.429447000	1.370775000	2.991915000
1	2.246235000	5.525544000	0.259925000
1	4.365743000	2.911795000	2.960551000
1	4.285260000	4.996160000	1.592107000

Cp*P{W(CO)$_5$}$_2$·TePh

74	-1.903961000	0.903184000	-1.080920000
6	-1.047411000	-1.785449000	1.695286000
6	-3.218073000	1.408052000	-2.526322000
6	-3.487758000	0.925232000	0.272568000
6	-0.385495000	1.093201000	-2.484952000
6	-2.378851000	-1.015009000	-1.796101000
6	-1.799519000	2.964933000	-0.822360000
6	-2.205166000	-1.189167000	2.484138000
6	-3.362166000	-1.776534000	2.079780000
6	-3.081360000	-2.760836000	1.024186000

6	-1.741378000	-2.809575000	0.793228000
6	-0.014313000	-2.423533000	2.638831000
6	-2.080198000	-0.307509000	3.698973000
6	-4.728088000	-1.576347000	2.662543000
6	-4.162851000	-3.582276000	0.390410000
6	-1.028513000	-3.773639000	-0.101966000
8	-3.971304000	1.653109000	-3.364271000
8	0.392193000	1.262357000	-3.309909000
8	-2.716228000	-1.967090000	-2.334659000
8	-1.846365000	4.113379000	-0.801474000
8	-4.418397000	1.082207000	0.926619000
1	0.480395000	-1.671841000	3.266867000
1	0.761059000	-2.961833000	2.088780000
1	-0.525321000	-3.140120000	3.297495000
1	-2.648482000	-0.732583000	4.539029000
1	-2.478811000	0.706251000	3.539164000
1	-1.044153000	-0.203154000	4.037710000
1	-5.472249000	-1.374109000	1.878614000
1	-4.758597000	-0.740351000	3.369224000
1	-5.065760000	-2.482248000	3.191334000
1	-4.902293000	-2.939462000	-0.112691000
1	-4.715896000	-4.160113000	1.147373000
1	-3.775807000	-4.285404000	-0.353550000
1	-0.399174000	-3.279755000	-0.853256000
1	-1.740284000	-4.406544000	-0.642157000
1	-0.367162000	-4.439865000	0.471141000
74	2.312918000	-1.313734000	-0.438203000
6	4.140436000	-1.772250000	-1.146789000
6	3.112643000	-0.966268000	1.438069000
6	1.469911000	-1.787038000	-2.277754000
6	2.774897000	0.595323000	-1.128574000
6	2.240984000	-3.316899000	0.059898000
8	5.192471000	-2.024914000	-1.550639000
8	3.164938000	1.572252000	-1.589675000
8	3.566956000	-0.829139000	2.487556000
8	2.335838000	-4.442156000	0.287116000
8	1.023387000	-2.089129000	-3.292869000
15	-0.138975000	-0.543552000	0.452351000
52	-0.087388000	1.643186000	1.812556000
6	1.682450000	2.724645000	1.256253000
6	1.605459000	3.785626000	0.343693000
6	2.881173000	2.466950000	1.937651000
6	2.735572000	4.569982000	0.097799000
6	4.005502000	3.256966000	1.683539000
6	3.935457000	4.305573000	0.762154000
1	0.677286000	4.011748000	-0.176317000
1	2.946127000	1.659904000	2.665363000
1	2.673622000	5.388764000	-0.619993000
1	4.937284000	3.049287000	2.211454000
1	4.816277000	4.917802000	0.563862000

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