Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

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Quantum Soldering of Individual Quantum Dots**

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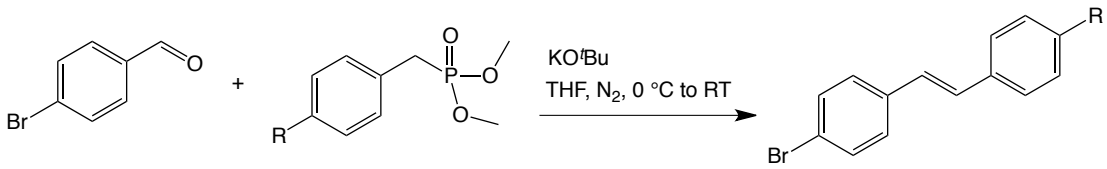
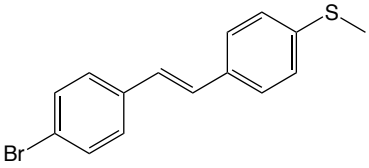
I. Synthetic Details
General Information

Chlorodiethylphosphine was purchased from Acros Organics. Selenium powder and dicobalt octacarbonyl were obtained from STREM Chemicals. Diethyl benzylphosphonate, 4-bromobenzaldehyde, potassium *tert*-butoxide, 4-bromothioanisole, 3-bromothioanisole, 4-(methylthio)benzylbromide, trimethylphosphite, 1,2,4-trichlorobenzene, and all other reagents and solvents were purchased from Aldrich. Dry and deoxygenated solvents were prepared by elution through a dual column solvent system (Glass Contour Solvent Systems). Unless otherwise noted, all reactions were carried out under nitrogen using standard schlenk techniques or in an argon-filled glovebox. Only the IR peaks in the range 4000-1500 cm^{-1} are reported.

General Horner-Wadsworth-Emmons reaction:

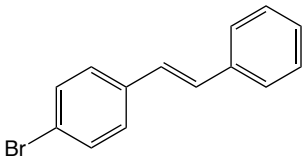


4-Bromo-4′-thiomethylstilbene: 4-Bromobenzaldehyde (0.89 g, 4.8 mmol) was dissolved in 40 mL of THF and cooled to 0 °C. Dimethyl-4-thiomethylbenzyl phosphonate[35] (1.18 g, 4.8 mmol) was added and the solution was stirred for 30 min. A solution of potassium *tert*-butoxide (0.62 g, 5.5 mmol) in 10 mL of THF was added dropwise to the cold reaction over 15 min. The reaction was stirred and warmed to RT overnight. In air, 50 mL of water was added and the mixture was poured into 50 mL of dichloromethane. The organic phase was extracted and the aqueous phase was washed twice with 10 mL of dichloromethane. The combined organic phase was washed with water and brine, dried with $MgSO_4$ and evaporated to dryness. The white solid was recrystallized at -30 °C from a mixture of toluene and hexanes. Yield: 1.35 g (92 %).



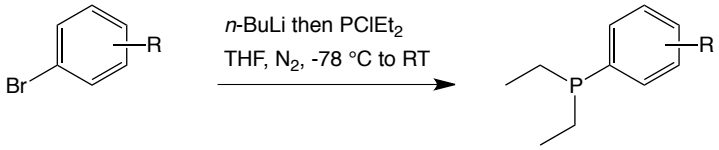
^{1}H NMR (300 MHz, [d_2-dichloromethane], 298 K): δ = 2.50 (3H, s), 7.00 (2H, m), 7.21-7.25 (2H, m), 7.32-7.48 (6H, m).
IR (ATR) $\bar{\nu}$ = 3079, 3015, 2917, 1903, 1834, 1628, 1590, 1551 cm^{-1}.

4-Bromostilbene: 4-Bromobenzaldehyde (2.10 g, 11.4 mmol) was dissolved in 50 mL of THF and cooled to 0 °C. Diethyl benzylphosphonate (2.61 g, 11.4 mmol) was added and the solution was stirred for 30 min. A solution of potassium *tert*-butoxide (1.40 g, 12.5 mmol) in 10 mL of THF was added dropwise to the cold reaction over 15 min. The reaction was stirred and warmed to RT overnight. In air, 50 mL of water was added and the mixture was poured into 50 mL of dichloromethane. The organic phase was extracted and the aqueous phase was washed twice with 10 mL of dichloromethane. The combined organic phase was washed with water and brine, dried with $MgSO_4$ and evaporated to dryness. The white solid was recrystallized at -30 °C from a mixture of toluene and hexanes. Yield: 2.44 g (83 %).



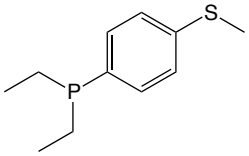
^{1}H NMR (300 MHz, [d_2-dichloromethane], 298 K): δ = 7.10 (2H, m), 7.26-7.31 (1H, m), 7.35-7.54 (8H, m).
IR (ATR) $\bar{\nu}$ = 3081, 3060, 3026, 2922, 1970, 1953, 1904, 1831, 1785, 1732, 1667, 1645, 1583 cm^{-1}.

General synthesis of the phosphine ligands:



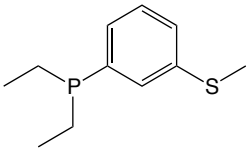
Diethyl-4-thiomethylphenylphosphine (L2): 4-Bromothioanisole (1.51g, 7.4 mmol) was dissolved in 50 mL of THF and cooled to -78 °C. *n*-Butyllithium (1.6 M in hexanes, 5.1 mL, 8.1 mmol) was added dropwise and the reaction was stirred for 45 min. Chlorodiethylphosphine (1.10 g, 8.8 mmol) in 10 mL of THF was added dropwise to the solution and the reaction was warmed

gradually to RT overnight. The solvent was removed under vacuum and 20 mL of toluene was added to the crude product. The mixture was filtered through a fine frit to remove LiCl and the solvent was once again removed under vacuum. The pale yellow oil obtained was distilled under vacuum at 110 °C to give a colorless oil. Yield: 1.32 g (84 %).



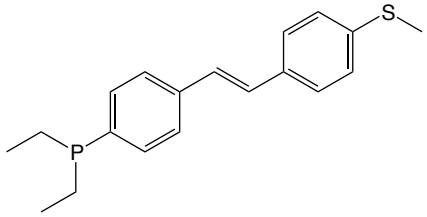
^{1}H NMR (400 MHz, [d_2-dichloromethane], 298 K): δ = 0.99 (6H, m), 1.66 (4H, m), 2.48 (3H, s), 7.23 (2H, m), 7.40 (2H, m).
^{31}P NMR (162 MHz, [d_2-dichloromethane], 298 K): δ = -16.
IR (ATR) $\bar{\nu}$ = 2957, 2927, 2871, 1885, 1634, 1579 cm^{-1}.

Diethyl-3-thiomethylphenylphosphine (L3): 3-Bromothioanisole (1.06 g, 5.2 mmol) was dissolved in 40 mL of THF and cooled to -78 °C. *n*-Butyllithium (1.6 M in hexanes, 3.6 mL, 5.7 mmol) was added dropwise and the reaction was stirred for 45 min. Chlorodiethylphosphine (0.78 g, 6.2 mmol) in 10 mL of THF was added dropwise to the solution and the reaction was warmed gradually to RT overnight. The solvent was removed under vacuum and 20 mL of toluene was added to the crude product. The mixture was filtered through a fine frit to remove LiCl and the solvent was once again removed under vacuum. The pale yellow oil obtained was distilled under vacuum at 110 °C to give a colorless oil. Yield: 0.78 g (71 %).



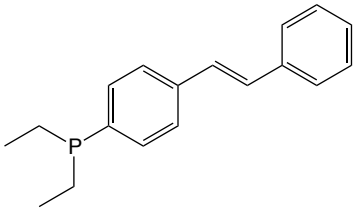
^{1}H NMR (500 MHz, [d_2-dichloromethane], 298 K): δ = 1.00 (6H, m), 1.68 (4H, m), 2.49 (3H, s), 7.20-7.29 (3H, m), 7.36-7.37 (1H, m).
^{31}P NMR (236 MHz, [d_2-dichloromethane], 298 K): δ = -14.
IR (ATR) $\bar{\nu}$ = 2959, 2931, 2876, 1635, 1574, 1562 cm^{-1}.

Diethyl-4'-thiomethyl-4-stilbenylphosphine (L4)*:* 4-Bromo-4′-thiomethylstilbene (1.16 g, 3.8 mmol) was dissolved in 50 mL of THF and cooled to -78 °C. *n*-Butyllithium (1.6 M in hexanes, 2.6 mL, 4.2 mmol) was added dropwise and the reaction was stirred for 45 min. Chlorodiethylphosphine (0.57 g, 4.6 mmol) in 10 mL of THF was added dropwise to the solution and the reaction was warmed gradually to RT overnight. The solvent was removed under vacuum and 20 mL of toluene was added to the crude product. The mixture was filtered through a fine frit to remove LiCl and the solvent was once again removed under vacuum. The white solid was recrystallized at -30 °C from a mixture of toluene and *n*-hexane. Yield: 1.00 g (84 %).



^{1}H NMR (400 MHz, [d_2-dichloromethane], 298 K): δ = 1.02 (6H, m), 1.70 (4H, m), 2.50 (3H, s), 7.10-7.11 (2H, m), 7.25 (2H, m), 7.45-7.51 (6H, m).
^{31}P NMR (162 MHz, [d_2-dichloromethane], 298 K): δ = -15.
IR (ATR) $\bar{\nu}$ = 3066, 3018, 2950, 2924, 2901, 2866, 2821, 1899, 1833, 1630, 1588, 1547 cm^{-1}.

Diethyl-4-stilbenylphosphine (L5): 4-Bromostilbene (0.49 g, 1.9 mmol) was dissolved in 40 mL of THF and cooled to -78 °C. *n*-Butyllithium (1.6 M in hexanes, 1.3 mL, 2.1 mmol) was added dropwise and the reaction was stirred for 45 min. Chlorodiethylphosphine (0.28 g, 2.3 mmol) in 10 mL of THF was added dropwise to the solution and the reaction was warmed gradually to RT overnight. The solvent was removed under vacuum and 20 mL of toluene was added to the crude product. The mixture was filtered through a fine frit to remove LiCl and the solvent was once again removed under vacuum. The white solid was recrystallized at -30 °C from *n*-hexane. Yield: 0.38 g (75 %).



[1]H NMR (400 MHz, [d_2-dichloromethane], 298 K): δ = 1.01 (6H, m), 1.70 (4H, m), 7.15 (2H, m), 7.27 (1H, m), 7.37 (2H, m), 7.46-7.55 (6H, m).
[31]P NMR (162 MHz, [d_2-dichloromethane], 298 K): δ = -15.
IR (ATR) $\bar{\nu}$ = 3064, 3020, 2955, 2927, 2912, 2869, 1950, 1915, 1828, 1597, 1576, 1548 cm^{-1}.

***General synthesis of the $Co_6Se_8L_6$ clusters**:*

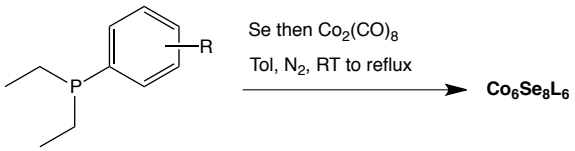
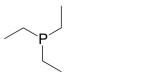
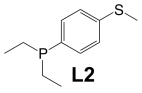
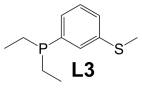
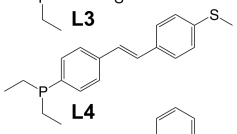
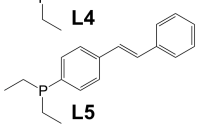


Table S1. List of the $Co_6Se_8\mathbf{L}_6$ clusters synthesized.

$Co_6Se_8L_6$	L
1	
2	 **L2**
3	 **L3**
4	 **L4**
5	 **L5**

***Cluster 1**:* Cluster **1** was synthesized according to a published procedure (*9*).
[1]H NMR (400 MHz, [d_6-benzene], 298 K): δ = 1.10 (36H, m), 1.96 (24H, m).
[31]P NMR (162 MHz, [d_6-benzene], 298 K): δ = 61 (broad peak).
The ^{31}P peak for compound **1** is very broad and we believe that it was wrongly assigned in ref. 2. We report the corrected shift here.
IR (ATR) $\bar{\nu}$ = 2966, 2925, 2877 cm^{-1}.

Cluster 2: Diethyl-4-thiomethylphenylphosphine (**L2**) (0.38 g, 1.8 mmol) was dissolved in 25 mL of toluene. Selenium powder (0.14 g, 1.8 mmol) was added and the suspension was stirred until the solid completely dissolved. Dicobalt octacarbonyl (0.14 g, 0.4 mmol), dissolved in 10 mL of toluene, was added to the solution and the reaction was heated to reflux overnight. The mixture was cooled down to room temperature and filtered through a fine frit. The dark brown solution was concentrated under vacuum and the product was precipitated with diethyl ether. Yield: 0.12 g (37 %).
Single crystals were grown by slow diffusion of *n*-hexane in a toluene solution of **2**.
[1]H NMR (400 MHz, [d_8-tetrahydrofuran], 298 K): δ = 0.86 (36H, m), 1.97 (24H, m), 2.50 (18H, s), 7.15 (12H, m), 7.28 (12H, m).
[31]P NMR (162 MHz, [d_8-tetrahydrofuran], 298 K): δ = 58 (broad peak).
IR (ATR) $\bar{\nu}$ = 3066, 2961, 2922, 2868, 1966, 1879, 1579, 1542 cm^{-1}.

***Cluster 3**:* Diethyl-3-thiomethylphenylphosphine (**L3**) (0.6 g, 2.8 mmol) was dissolved in 40 mL of toluene. Selenium powder (0.22 g, 2.8 mmol) was added and the suspension was stirred until the solid completely dissolved. Dicobalt octacarbonyl (0.22 g, 0.6 mmol), dissolved in 10 mL of toluene, was added to the solution and the reaction was heated to reflux overnight. The mixture was cooled

down to room temperature and filtered through a fine frit. The solvent was removed under vacuum to give a dark brown oil. Large black single crystals of **3** were grown from a mixture of diethyl ether and *n*-hexane. Yield: 0.23 g (46 %).
^{1}H NMR (400 MHz, [d_8-tetrahydrofuran], 298 K): δ = 0.88 (36H, m), 1.95 (24H, m), 2.48 (18H, s), 7.09-7.13 (12H, m), 7.16-7.20 (6H, m), 7.34 (6H, m).
^{31}P NMR (162 MHz, [d_8-tetrahydrofuran], 298 K): δ = 58 (broad peak).
IR (ATR) $\bar{\nu}$ = 3038, 2964, 2926, 2870, 2727, 1954, 1859, 1740, 1669, 1570, 1561 cm^{-1}.

Cluster 4*:* Diethyl-4'-thiomethyl-4-stilbenylphosphine (**L4**) (223 mg, 0.71 mmol) was dissolved in 40 mL of toluene. Selenium powder (56 mg, 0.71 mmol) was added and the suspension was stirred until the solid completely dissolved. Dicobalt octacarbonyl (56 mg, 0.16 mmol), dissolved in 5 mL of toluene, was added to the solution and the reaction was heated to reflux overnight. The hot mixture was filtered through a fine frit. The dark brown solution was concentrated under vacuum and the product was precipitated with diethyl ether. Yield: 102 mg (65 %).
Single crystals were grown by slow evaporation of a toluene solution of **4**.
^{1}H NMR (400 MHz, [d_8-tetrahydrofuran], 298 K): δ = 0.89 (36H, m), 2.06 (24H, m), 2.48 (18H, s), 7.13 (12H, s), 7.20 (12H, m), 7.32-7.43 (36H, m).
^{31}P NMR (162 MHz, [d_8-tetrahydrofuran], 298 K): δ = 58 (broad peak).
IR (ATR) $\bar{\nu}$ = 3018, 2963, 2921, 2872, 1629, 1586, 1545 cm^{-1}.

Cluster 5*:* Diethyl-4-stilbenylphosphine (**L5**) (300 mg, 1.12 mmol) was dissolved in 40 mL of toluene. Selenium powder (88 mg, 0.71 mmol) was added and the suspension was stirred until the solid completely dissolved. Dicobalt octacarbonyl (88 mg, 0.26 mmol), dissolved in 10 mL of toluene, was added to the solution and the reaction was heated to reflux overnight. The mixture was cooled down to room temperature and filtered through a fine frit. The dark brown solution was concentrated under vacuum and black single crystals of **5** were grown by slow evaporation of the solution. Yield: 125 mg (56 %).
^{1}H NMR (400 MHz, [d_8-tetrahydrofuran], 298 K): δ = 0.90 (36H, m), 2.06 (24H, m), 7.19-7.22 (18H, m), 7.28-7.31 (12H, m), 7.35-7.39 (12H, m), 7.44-7.49 (24H, m).
^{31}P NMR (162 MHz, [d_8-tetrahydrofuran], 298 K): δ = 56 (broad peak).
IR (ATR) $\bar{\nu}$ = 3075, 3056, 3025, 2962, 2931, 2907, 2874, 1942, 1875, 1823, 1633, 1597, 1575, 1551 cm^{-1}.

II. Instrumentation Details.

All ^{1}H and ^{31}P NMR were recorded on a Bruker DRX300 (300 MHz), Bruker DRX400 (400 MHz), or Bruker DMX500 (500 MHz) spectrometer. Infrared (IR) spectra were obtained using a Perkin Elmer Spectrum 400 FTIR spectrometer using a PIKE ATR attachment. Absorption spectra were taken on a Shimadzu UV-1800 spectrophotometer. Electrochemistry was performed using a CHI600c potentiostat and analyzed using the CHI600c electrochemical analyzer software package. Single crystal X-ray diffraction data were collected on a Bruker SMART CCD APEX II diffractometer using a fine-focus sealed-tube graphite monochromator Cu K_{α} source (λ = 1.54178 Å). The conductance measurements were performed using a home-built modified scanning tunneling microscope (STM) that has been previously described.[36] Sub-angstrom level control of the tip-substrate distance was achieved using a commercially available single-axis piezoelectric positioner (Nano-P15, Mad City Labs). The STM was controlled using a custom program using IgorPro (Wavemetrics, Inc.).

III. Conductance Measurements and Additional Data.

General Information

The conductance of each molecule was measured using the STM-based break-junction technique, where an Au tip (Alfa Aesar, 99.999%) cut to be sharp is brought in and out of contact with a substrate of ~100 nm of gold (Alfa Aesar, 99.999%) evaporated onto cleaved mica disks. The substrate is mounted on a piezoelectric positioner (Mad City Labs), so that sub-angstrom resolution in position is achieved. During the entire break junction procedure, a bias (500 mV for the molecular connector and 750 mV for the complex) is applied between the tip and the substrate while the current is measured (Keithley 428-Prog). Piezo control and data collection were performed using a National Instruments PXI Chassis System (with PXI-4461, PXI-6289) at 40 kHz, and driven and managed with a custom-program using Igor Pro (Wavemetrics, Inc.).

The experimental set-up is kept under ambient. For each experiment, the substrate is cleaned under UV/Ozone for 15 minutes prior to use. For every conductance trace measurement, the STM tip is first brought into hard contact with the substrate to achieve a conductance greater than ~ 10 G_0. At this point, the junction electrodes are pulled apart at a speed of 15 nm/s for 0.25 seconds. Conductance is measured as a function of tip-sample displacement to generate conductance traces. For each tip/substrate pair, at least one set of 1,000 traces of clean gold breaks is collected to ensure the system is clean. Then, the target molecule, dissolved in 1,2,4-trichlorobenzene (1 mM) is deposited and over 5,000 conductance traces are collected for each of the molecules reported here. One-dimensional conductance histograms are created using every measured trace.

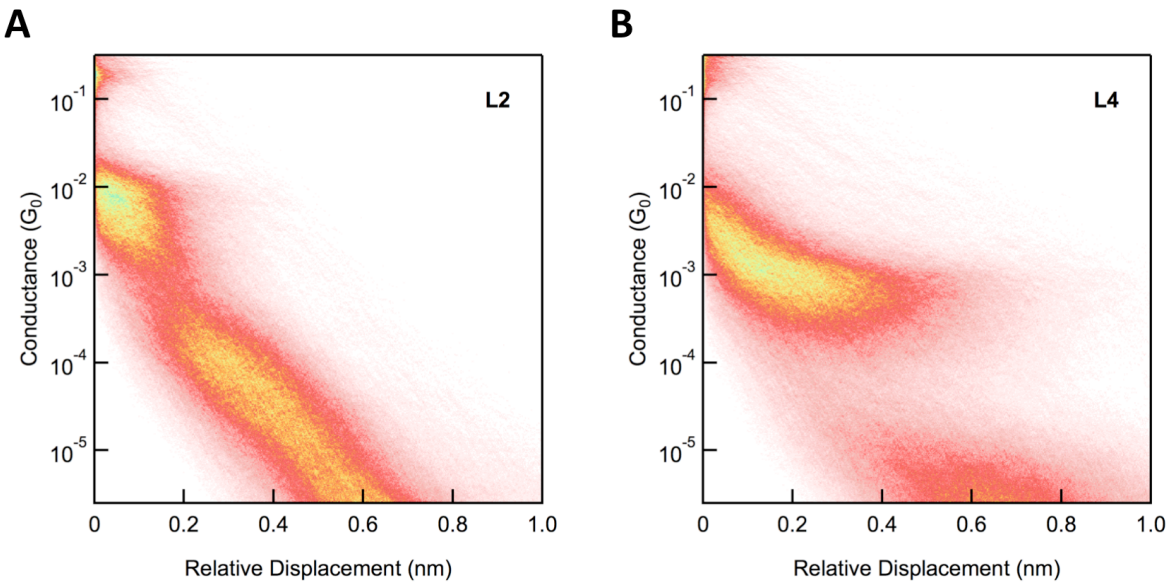


Figure S1. Two-dimensional histograms showing ligand conductance as a function of STM tip-sample displacement for compounds (**A**) **L2** and (**B**) **L4**. These histograms are generated using a logarithmic binning with 10 bins/decade. The displacement dimension was binned linearly. The color scale indicates the average number of counts per trace in a given conductance-displacement bin.

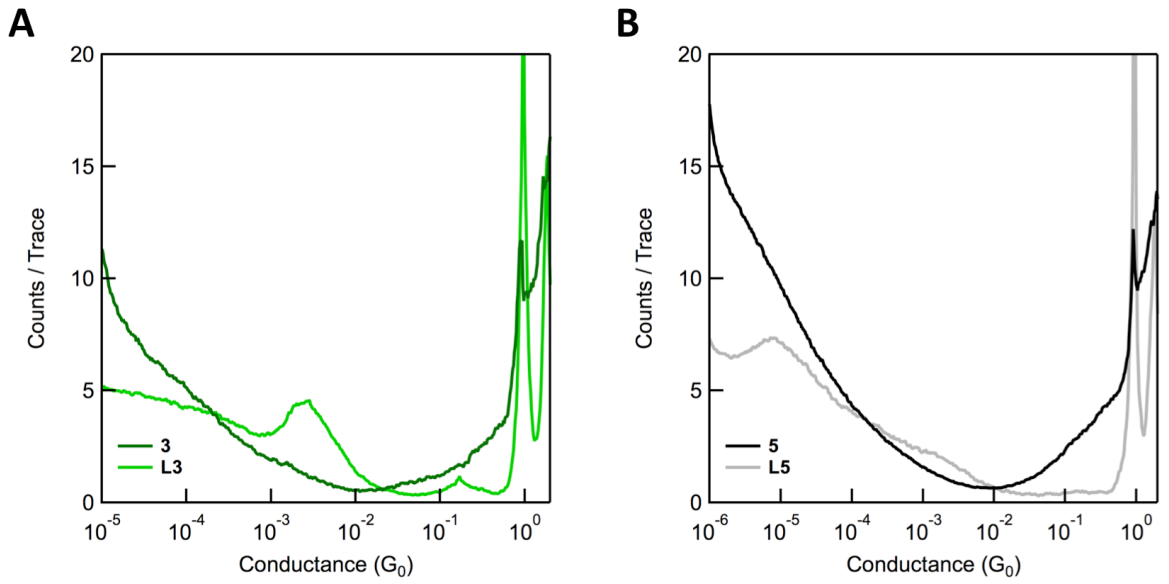


Figure S2. One-dimensional logarithm-binned conductance histograms of (**A**) **3** (dark green) and **L3** (light green) and (**B**) **5** (black) and **L5** (grey). Bin size is 100/decade.

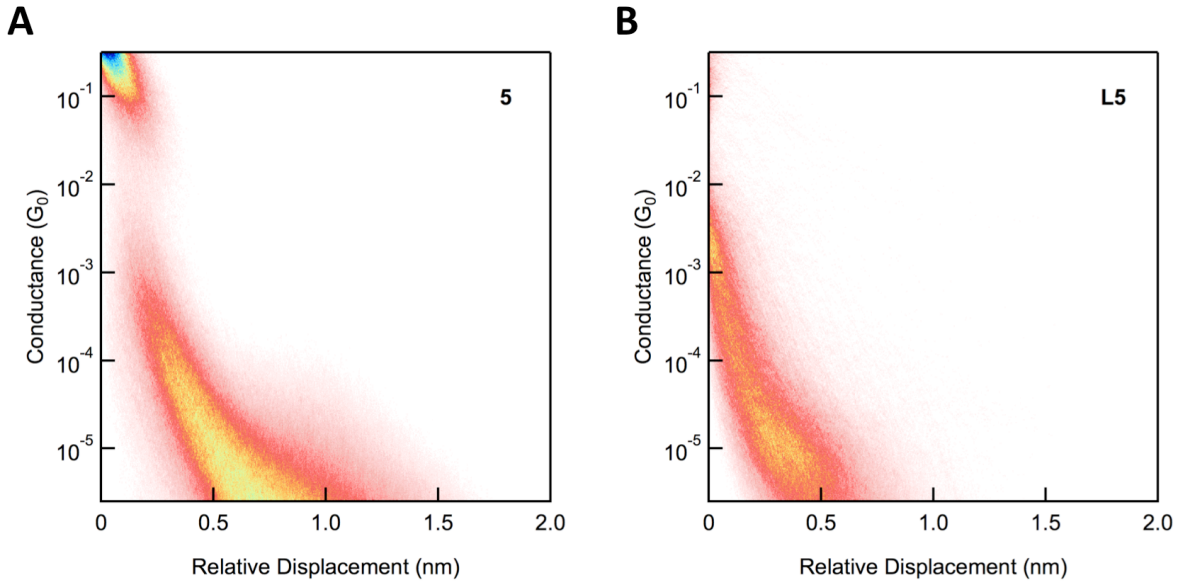


Figure S3. Two-dimensional histograms showing conductance as a function of STM tip-sample displacement for compounds (**A**) **5** and (**B**) **L5**. These histograms are generated using a logarithmic binning with 10 bins/decade. The displacement dimension was binned linearly. The color scale indicates the average number of counts per trace in a given conductance-displacement bin.

IV. UV-Vis Absorption Spectroscopy

General Information

All spectra were taken under nitrogen in a 1-cm quartz cuvette following a recording of the background spectrum.

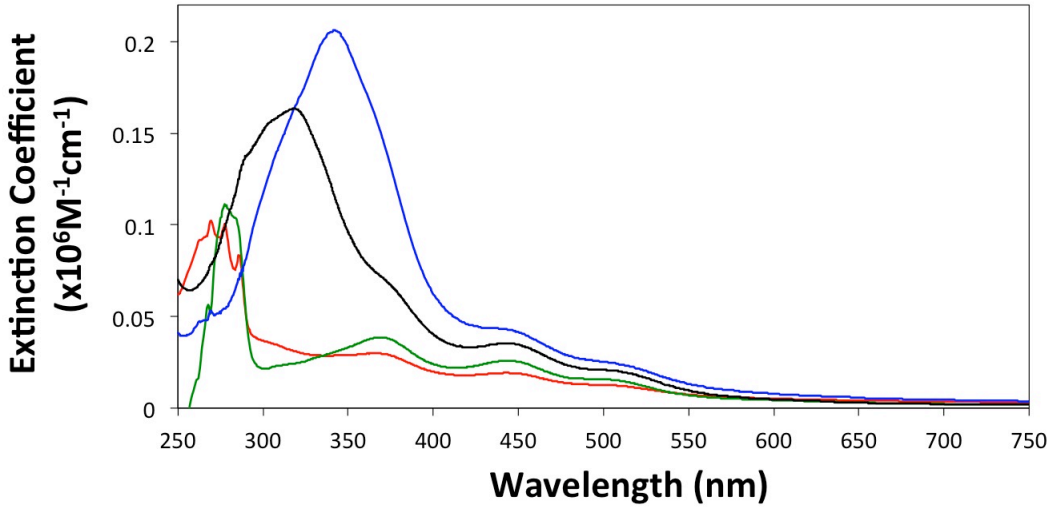


Figure S4. UV-vis spectra of clusters **2**-**5** taken in dry and degassed THF with the following concentrations: **2**, 5.5 μM (red); **3**, 5.8 μM (green); **4**, 3.3 μM (blue); **5**, 3.3 μM (black).

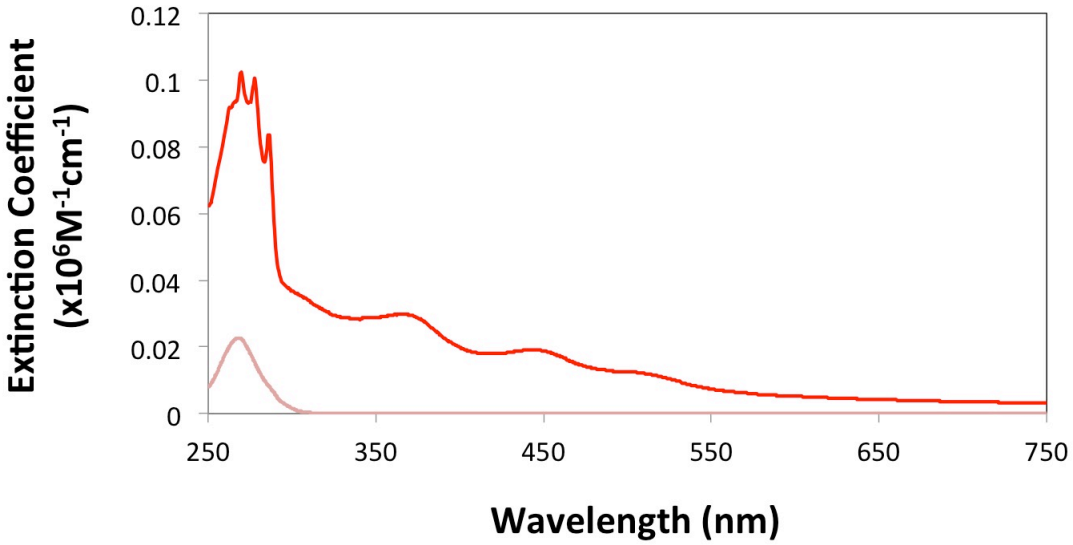


Figure S5. UV-vis spectra taken in dry and degassed THF with the following concentrations: **2**, 5.5 μM (red); **L2**, 26.0 μM (pink).

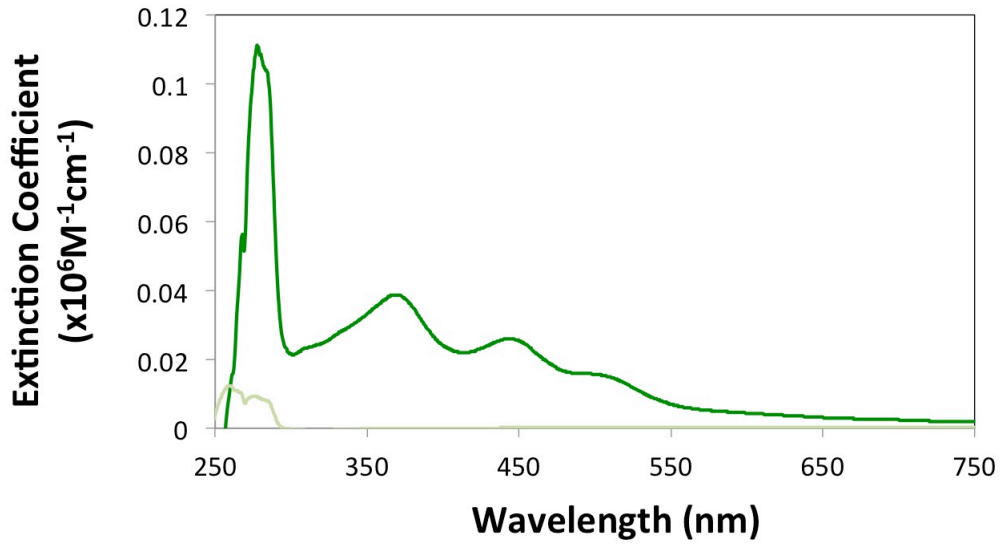


Figure S6. UV-vis spectra taken in dry and degassed THF with the following concentrations: **3**, 5.8 μM (dark green); **L3**, 51.0 μM (light green).

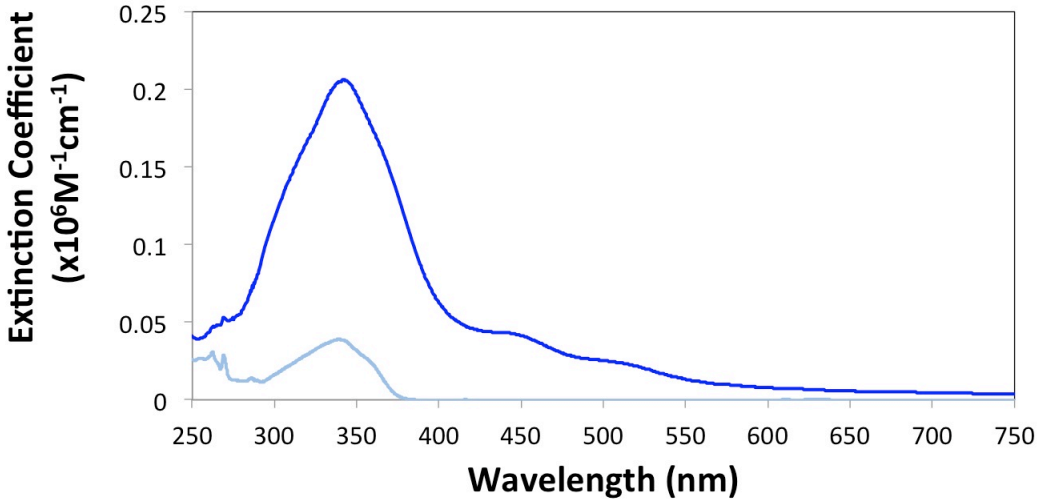


Figure S7. UV-vis spectra taken in dry and degassed THF with the following concentrations: **4**, 3.3 μM (dark blue); **L4**, 4.1 μM (blue).

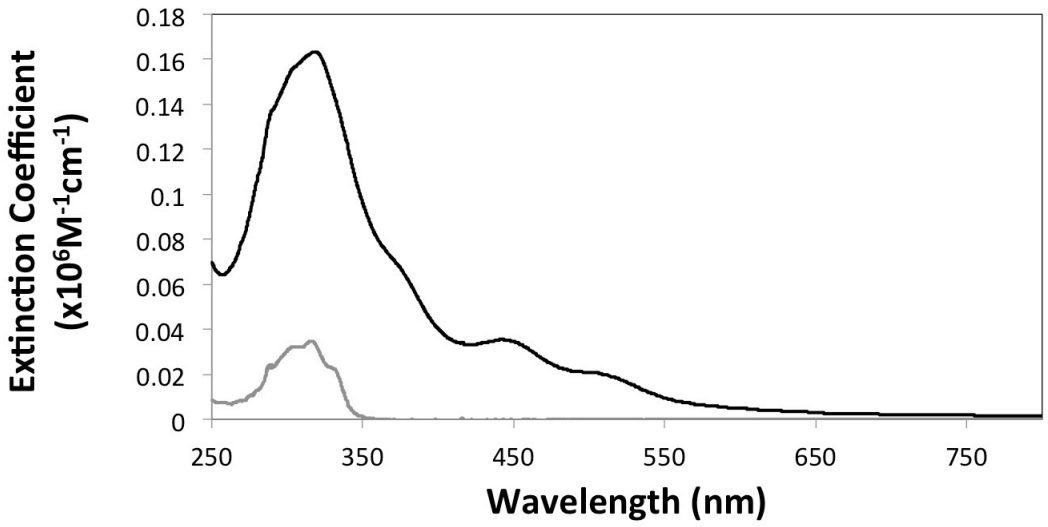


Figure S8. UV-vis spectra taken in dry and degassed THF with the following concentrations: **5**, 3.3 μM (black); **L5**, 2.9 μM (gray).

V. Electrochemistry

General Information

A solution of clusters **2**-**5** in degassed, anhydrous dichloromethane containing 0.1 M of supporting electrolyte, tetrabutylammonium hexafluorophosphate ($TBAPF_6$) was used in a single cell. The measurements were carried out under nitrogen in a cell with a glassy carbon working electrode, a platinum wire counter electrode and a Ag^+/AgCl reference electrode with a scan rate of 0.1 V/s. The potentials are reported against a Ag^+/AgCl reference.

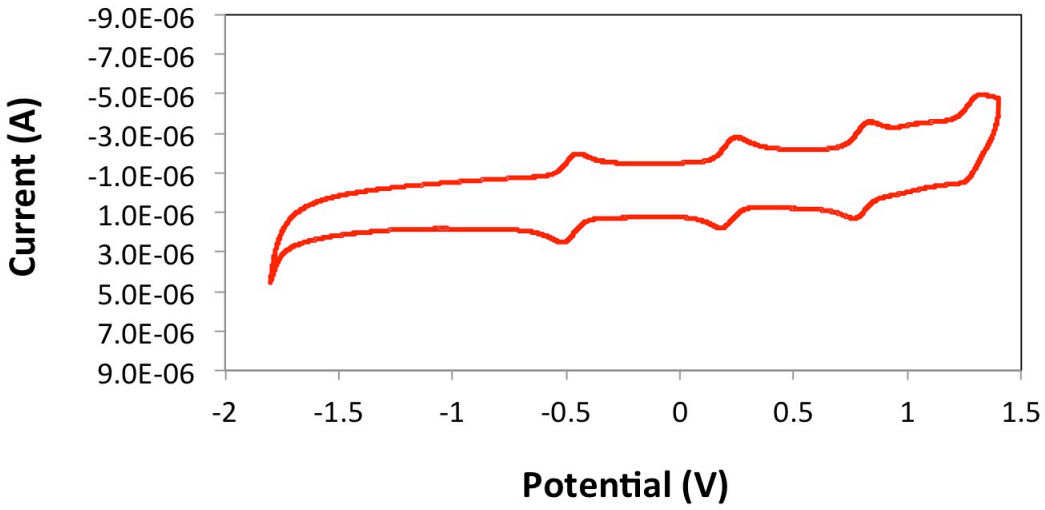


Figure S9. CV trace of **2** in 0.1 M $TBAPF_6$ in dichloromethane vs. Ag^+/AgCl.

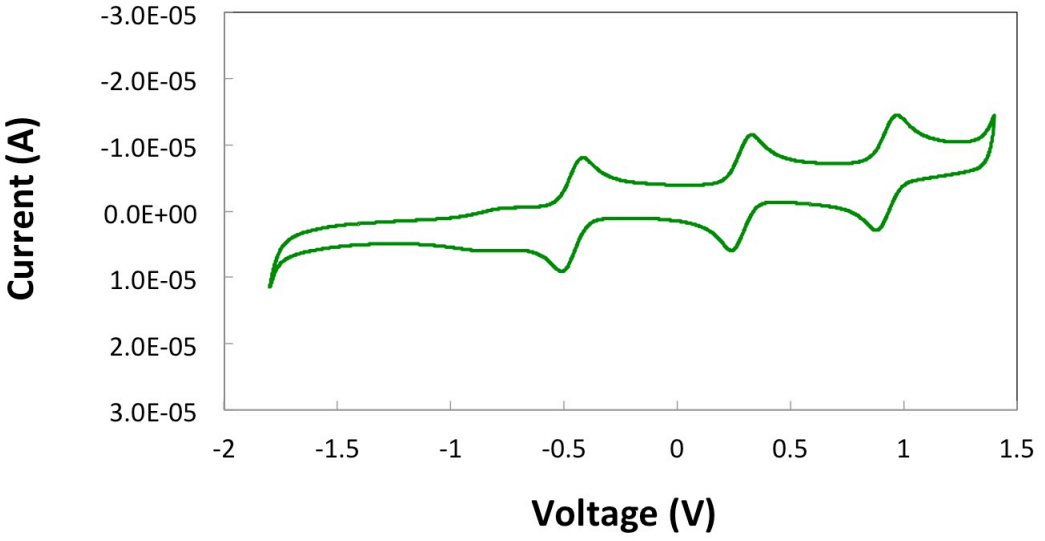


Figure S10. CV trace of **3** in 0.1 M $TBAPF_6$ in dichloromethane.

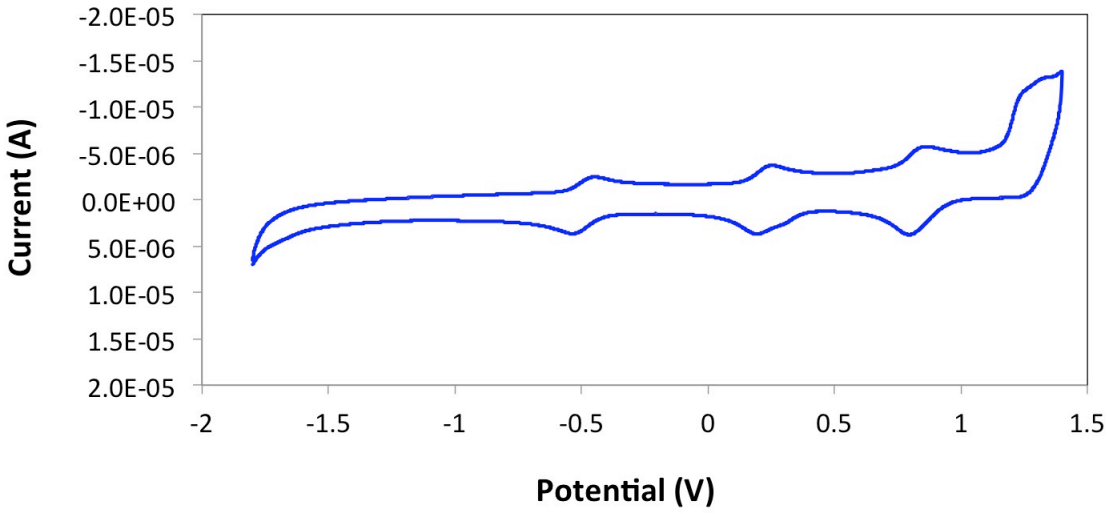


Figure S11. CV trace of **4** in 0.1 M $TBAPF_6$ in dichloromethane.

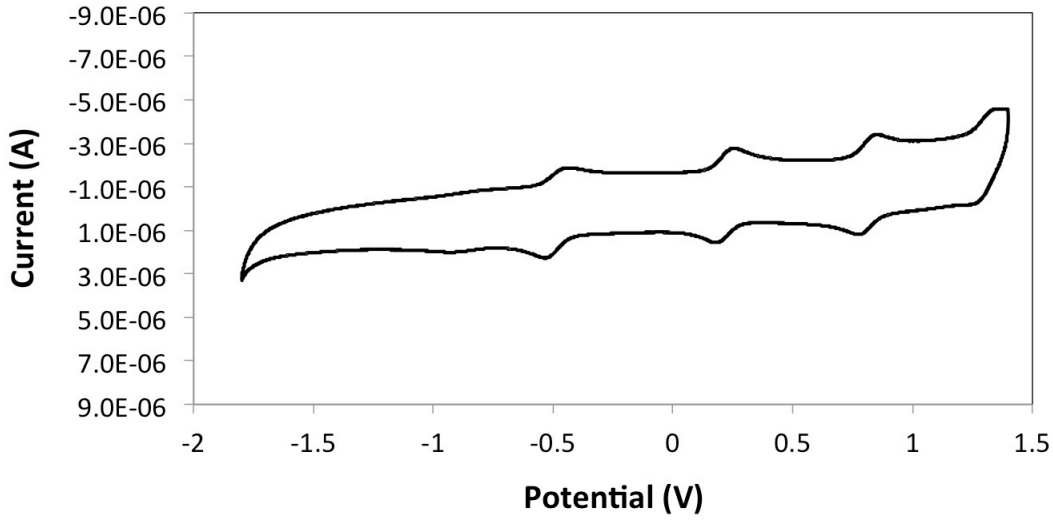


Figure S12. CV trace of **5** in 0.1 M $TBAPF_6$ in dichloromethane.

V. Single Crystal X-ray diffraction

General Information

Crystals of **1** suitable for X-ray diffraction were grown by slow diffusion of *n*-hexane in a toluene solution of the compound. All measurements were made on a Bruker SMART CCD APEX II diffractometer[37] using a fine-focus sealed-tube graphite monochromator Cu K_α source (λ = 1.54178 Å). Of the 12,986 reflections that were collected, 1,958 were unique (R_{int} = 0.039); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT software package.[38] Data were corrected for absorption effects using a multi-scan technique (SADABS)[39] and numerical face-indexing with max and min transmission coefficients of 0.2095 and 0.1663, respectively. The structure was solved using SHELXTL.[40] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were found in electron-density difference maps, but placed in idealized positions and allowed to ride on their respective C atoms. The final cycle of full-matrix least-squares refinement on F^2 was based on 1,962 reflections and 88 variable parameters and converged. Cambridge Crystallographic Data Centre deposition number: 894787

Crystals of **2** suitable for X-ray diffraction were grown by slow diffusion of *n*-hexane in a toluene solution of the compound. All measurements were made on a Bruker SMART CCD APEX II diffractometer[37] using a fine-focus sealed-tube graphite monochromator Cu K_α source (λ = 1.54178 Å). Of the 40,988 reflections that were collected, 7,134 were unique (R_{int} = 0.049); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT software package.[38] Data were corrected for absorption effects using a multi-scan technique (SADABS)[39] and numerical face-indexing with max and min transmission coefficients of 0.228 and 0.141, respectively. The structure was solved using SHELXTL.[40] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were found in electron-density difference maps, but placed in idealized positions and allowed to ride on their respective C atoms. The final cycle of full-matrix least-squares refinement on F^2 was based on 7,134 reflections and 425 variable parameters and converged. Cambridge Crystallographic Data Centre deposition number: 894788

Crystals of **3** suitable for X-ray diffraction were grown from a mixture of diethyl ether and *n*-hexane. All measurements were made on a Bruker SMART CCD APEX II diffractometer[37] using a fine-focus sealed-tube graphite monochromator Cu K_α source (λ = 1.54178 Å). Of the 21,117 reflections that were collected, 7,059 were unique (R_{int} = 0.049); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT software package.[38] Data were corrected for absorption effects using a multi-scan technique (SADABS)[39] and numerical face-indexing with max and min transmission coefficients of 0.158 and 0.054, respectively. The structure was solved using SHELXTL.[40] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were found in electron-density difference maps, but placed in idealized positions and allowed to ride on their respective C atoms. The final cycle of full-matrix least-squares refinement on F^2 was based on 7,059 reflections and 424 variable parameters and converged. Cambridge Crystallographic Data Centre deposition number: 894789

Crystals of **4** suitable for X-ray diffraction were grown by slow evaporation of a toluene solution of the compound. All measurements were made on a Bruker SMART CCD APEX II diffractometer[37] using a fine-focus sealed-tube graphite monochromator Cu K_α source (λ = 1.54178 Å). Of the 56,108 reflections that were collected, 11,178 were unique (R_{int} = 0.043); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT software package.[38] Data were corrected for absorption effects using a multi-scan technique (SADABS)[39] and numerical face-indexing with max and min transmission coefficients of 0.450 and 0.116, respectively. The structure was solved using SHELXTL.[40] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were found in electron-density difference maps, but placed in idealized positions and allowed to ride on their respective C atoms. The final cycle of full-matrix least-squares refinement on F^2 was based on 11,178 reflections and 724 variable parameters and converged. Cambridge Crystallographic Data Centre deposition number: 894790

Crystals of **5** suitable for X-ray diffraction were grown by slow evaporation of a toluene solution of the compound. All measurements were made on a Bruker SMART CCD APEX II diffractometer[37] using a fine-focus sealed-tube graphite monochromator Cu K_α source (λ = 1.54178 Å). Of the 24,900 reflections that were collected, 3,251 were unique (R_{int} = 0.046); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT software package.[38] Data were corrected for absorption effects using a multi-scan technique (SADABS)[39] and numerical face-indexing with max and min transmission coefficients of 0.393 and 0.160, respectively. The structure was solved using SHELXTL.[40] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were found in electron-density difference maps, but placed in idealized positions and allowed to ride on their respective C atoms. The final cycle of full-matrix least-squares refinement on F^2 was based on 3,251 reflections and 195 variable parameters and converged. Cambridge Crystallographic Data Centre deposition number: 894791.

Table S2. Selected crystallographic data for clusters **1**-**3**.

Compound	**1**	**2**	**3**
Formula	$C_{36}H_{90}Co_6P_6Se_8$	$C_{66}H_{102}Co_6P_6S_6Se_8$	$C_{66}H_{102}Co_6P_6S_6Se_8$
MW	1694.16	2258.98	2258.98
Lattice type	Hexagonal	Monoclinic	Triclinic
Space group	$R\bar{3}$	$C2/c$	$P\bar{1}$
a (Å)	17.1179(2)	27.8535(4)	11.7100(4)
b (Å)	17.1179(2)	16.8649(2)	13.1148(4)
c (Å)	19.5825(3)	21.5166(2)	15.1233(5)
α (°)	90	90	73.504(1)
β (°)	90	125.605(1)	74.179(2)
γ (°)	120	90	68.884(1)
V (Å^3)	4969.35(11)	8217.8(2)	2039.40(12)
Z value	3	4	1
D_{calc} (g cm^{-3})	1.698	1.826	1.839
T (K)	298	100	100
GOF on F^2	1.07	1.03	1.03
R_1 [$F^2 > 2\sigma(F^2)$]	0.031	0.033	0.054
wR_2 (all data)	0.086	0.080	1.151

Table S3. Selected crystallographic data for compounds **4** and **5**.

Compound	**4**	**5**
Formula	$C_{114}H_{138}Co_6P_6S_6Se_8$, $2(C_7H_8)$	$C_{108}H_{126}Co_6P_6Se_8$
MW	3056.02	2595.17
Lattice type	Monoclinic	Hexagonal
Space group	$P2_1/c$	$R\bar{3}$
a (Å)	11.8387(2)	17.7839(2)
b (Å)	45.8633(7)	17.7839(2)
c (Å)	11.7945(2)	28.5185(4)
α (°)	90	90
β (°)	93.493(7)	90
γ (°)	90	120
V (Å^3)	6392.07(18)	7811.08(17)
Z value	2	3
D_{calc} (g cm^{-3})	1.588	1.655
T (K)	100	100
GOF on F^2	1.23	1.06
R_1 [$F^2 > 2\sigma(F^2)$]	0.045	0.045
wR_2 (all data)	0.094	0.106

VII. DFT Calculations

General Information. All density functional calculations were performed using Jaguar.[41] Geometries were optimized, orbitals were calculated, and energies were determined all at the B3LYP/6-31G** level. We report final energies, orbital energies, and final geometries for $Co_6Se_8(PMe_3)_5L$ and $Co_6Se_8(PMe_3)_4\mathbf{L}_2$ for **L** = dimethyl-4-thiomethylphenylphosphine (**L2**), dimethyl-3-thiomethylphenylphosphine (**L3**), and diethyl-4'-thiomethyl-4-stilbenylphosphine (**L4**) below.

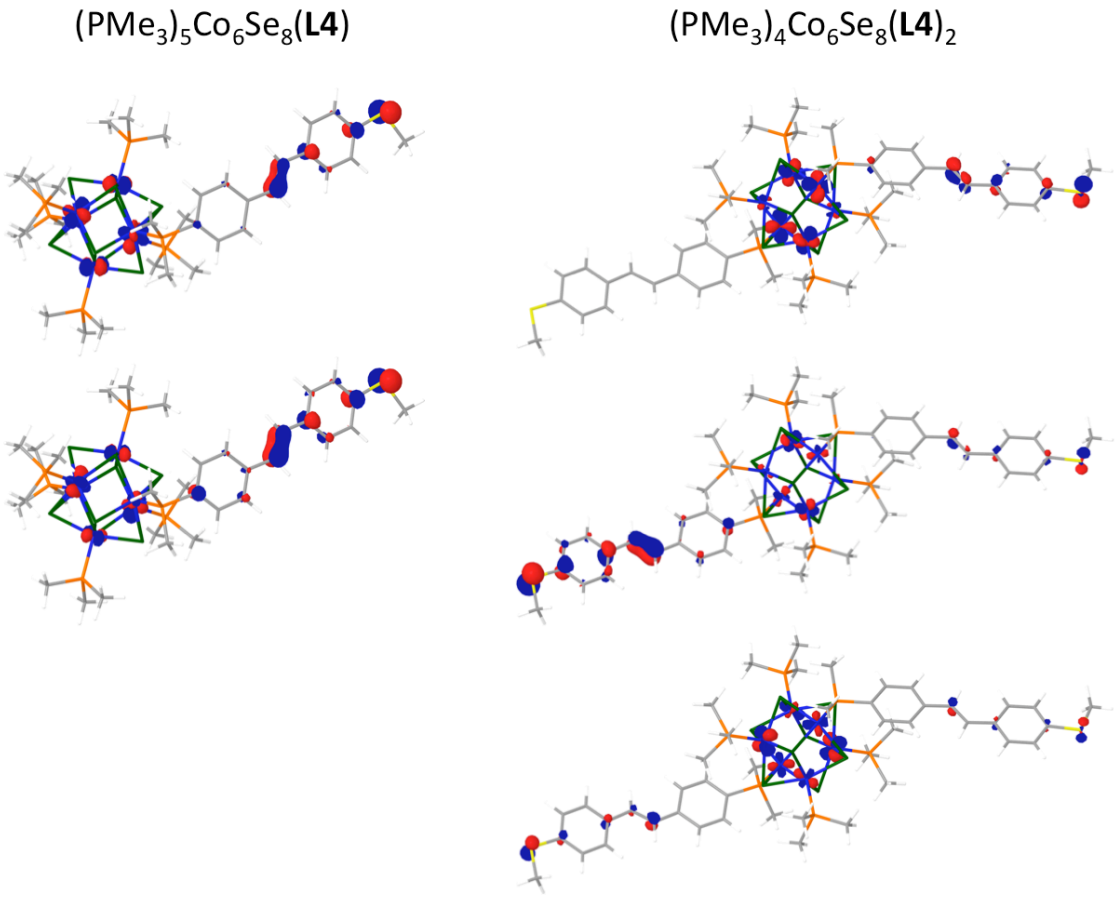


Figure S13. Model computational studies of cluster **4** using density functional theory. The orbitals associated with the sulfur pπ lone pairs for the models $(PMe_3)_5Co_6Se_8$(**L4**) and $(PMe_3)_4Co_6Se_8$(**L4**)$_2$ are shown.

VIII. References

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[41] Schrodinger, *Jaguar*. Version 7.8. Schrodinger LLC. New York, NY, USA **2010**.

IX. DFT data

co6se8_pme3_5_4-thiomethylphenyldimethylphosphine

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.............   10478.27273560042
   (E)  Total one-electron terms.....  -27252.17894854997
   (I)  Total two-electron terms.....   12433.05230367432
   (J)    Coulomb....................   12856.67857904475
   (K)    Exchange+Correlation.......    -423.62627537043
   (L)  Electronic energy............  -14819.12664487565  (E+I)
   (N)  Total energy.................   -4340.85390927524  (A+L)

 SCFE: SCF energy: DFT(b3lyp)     -4340.85390927524 hartrees

 HOMO energy:    -0.15760
 LUMO energy:    -0.05577

  Orbital energies (hartrees):
   -88.86471   -77.09488   -77.09114   -77.09070   -77.09070   -77.09049
   -77.09003   -10.21822   -10.21402   -10.18985   -10.18829   -10.18769
   -10.18713   -10.18660   -10.17453   -10.17331   -10.17303   -10.17292
   -10.17291   -10.17288   -10.17282   -10.17276   -10.17269   -10.17234
   -10.17233   -10.17213   -10.17162   -10.17150   -10.17125   -10.17096
   -10.17074    -7.94067    -6.57165    -6.56836    -6.56795    -6.56792
    -6.56774    -6.56726    -5.90517    -5.90102    -5.89473    -4.73367
    -4.73343    -4.73046    -4.73019    -4.73017    -4.72978    -4.72976
    -4.72975    -4.72973    -4.72957    -4.72954    -4.72909    -4.72906
    -4.72725    -4.72685    -4.72682    -4.72665    -4.72617    -3.70175
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    -2.39196    -2.39192    -2.39179    -2.39164    -2.39157    -2.39137
    -2.39118    -2.39108    -2.39092    -2.39091    -2.39086    -0.86186
    -0.80222    -0.76413    -0.76364    -0.76353    -0.76328    -0.76276
    -0.76044    -0.74670    -0.72493    -0.68850    -0.68794    -0.68757
    -0.68753    -0.68746    -0.68700    -0.68695    -0.68653    -0.68636
    -0.68613    -0.68567    -0.65434    -0.64349    -0.61509    -0.61446
    -0.61407    -0.60638    -0.59411    -0.59144    -0.59098    -0.58660
    -0.57967    -0.55126    -0.53767    -0.53722    -0.53652    -0.53649
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    -0.42127    -0.42116    -0.42103    -0.42075    -0.42030    -0.41146
    -0.40152    -0.40018    -0.39962    -0.39935    -0.39922    -0.39893
    -0.39862    -0.39793    -0.39780    -0.39762    -0.39650    -0.39048
    -0.38144    -0.38088    -0.38080    -0.38063    -0.38045    -0.38007
    -0.37147    -0.35264    -0.33659    -0.33346    -0.33228    -0.33180
    -0.33174    -0.33156    -0.33144    -0.33126    -0.33065    -0.33050
    -0.33028    -0.32980    -0.32739    -0.32670    -0.31898    -0.31680
    -0.30999    -0.30896    -0.30770    -0.29389    -0.28508    -0.28270
    -0.28242    -0.28130    -0.27996    -0.27919    -0.27841    -0.27780
    -0.27772    -0.27580    -0.27522    -0.27037    -0.25375    -0.25301
    -0.25254    -0.25046    -0.23824    -0.23709    -0.23695    -0.23582
    -0.23070    -0.23029    -0.22927    -0.22796    -0.22754    -0.22710
    -0.22688    -0.22602    -0.22082    -0.21529    -0.21508    -0.20716
```

-0.19883	-0.19640	-0.19595	-0.19179	-0.19140	-0.18963
-0.18163	-0.18020	-0.17980	-0.17004	-0.16064	-0.16005
-0.15760	-0.05577	-0.05310	-0.05259	-0.04538	-0.04439
-0.03594	-0.03508	-0.03423	-0.03171	-0.03144	

final geometry:

		angstroms	
atom	x	y	z
C1	-0.1983799660	0.1077222728	-0.0797445734
P2	0.0736513745	0.2041252298	1.7430802332
C3	1.8977465461	0.4653161608	1.8286337504
Co4	-1.1714100834	1.6361894579	2.8277795841
Se5	-1.8580094080	0.3397805073	4.7584415228
Co6	-3.8384688640	1.5517150688	4.0767069769
Se7	-3.8608764965	2.5840942297	6.2617049979
Co8	-1.5201438621	2.5681429733	5.6236099270
Se9	-1.5173457857	4.9844897900	5.7985296282
Co10	-3.6310349173	4.4486357284	4.7336055115
Se11	-5.2575216816	3.3629524765	3.3251618393
Co12	-3.2803415810	3.4959499724	1.9385352708
Se13	-3.2782352204	1.0807232147	1.7690673052
Co14	-0.9605916452	4.5188296238	3.4846616167
Se15	0.4622508607	2.7091464899	4.2425882259
P16	0.4982101235	6.1274261089	3.2318041216
C17	2.0981752902	5.9345152569	4.1297420319
Se18	-2.9382043890	5.7291428335	2.7940208000
Se19	-0.9430259592	3.4934221213	1.2963443515
C20	-0.0354500598	7.8050014424	3.7861530228
C21	1.0624897503	6.4695940812	1.5092741842
P22	-4.2854570884	3.9079754339	0.0446032380
C23	-4.9788898115	5.6038976151	-0.1640142575
C24	-3.2672963465	3.7133073026	-1.4810251677
C25	-5.7514196505	2.8580903157	-0.3475257324
P26	-4.8078026988	5.9747015448	5.7776531573
P27	-0.5360255999	2.1539902436	7.5305986435
C28	0.9865049074	3.1343426465	7.8867798698
C29	0.0639197705	0.4302058307	7.7976687596
C30	-1.5369118781	2.4537664094	9.0505734195
C31	-0.0843408093	-1.5661720326	2.2372386813
P32	-5.2860012664	-0.0659094065	4.3271182588
C33	-6.8921581945	0.1265277720	3.4411806314
C34	-5.8325244890	-0.4228489889	6.0521879398
C35	-4.7462271276	-1.7367744805	3.7582017691
H36	0.5533191614	-2.2017785890	1.6126088479
H37	0.1956924312	-1.6786317294	3.2867329668
H38	-1.1265901140	-1.8763347562	2.1321085781
H39	2.4253528741	-0.2813899751	1.2246448467
H40	2.1334666673	1.4671240762	1.4618886200
H41	2.2281339223	0.4017687050	2.8674577906
H42	0.4719475448	-0.6320064966	-0.5314781194
H43	-1.2369741712	-0.1679511648	-0.2749498331
H44	-0.0153227444	1.0896809182	-0.5215613219
H45	-0.9442685371	2.2580106671	9.9512349111

H46	-1.8787732668	3.4913533025	9.0543392016
H47	-2.4180787838	1.8089050762	9.0397064809
H48	0.5652023305	0.3392988654	8.7678159834
H49	-0.7795522319	-0.2617335528	7.7505103784
H50	0.7599827337	0.1650951752	6.9983434505
H51	1.4035297600	2.8596253837	8.8620807627
H52	1.7248595491	2.9478969458	7.1039051519
H53	0.7387030201	4.1980573288	7.8782634565
H54	-6.5273923536	-1.2698476523	6.0728323506
H55	-4.9570584686	-0.6511254496	6.6646854241
H56	-6.3153105972	0.4613568105	6.4735095149
H57	-5.5407811518	-2.4745015814	3.9165541972
H58	-4.4938908184	-1.6900739993	2.6965068144
H59	-3.8518184319	-2.0334372688	4.3103185613
H60	-7.5327314422	-0.7475544606	3.6031515412
H61	-7.3981801027	1.0276909551	3.7934275603
H62	-6.6971116656	0.2445898746	2.3726640784
H63	2.7396594113	6.8088830092	3.9726171705
H64	1.8964272211	5.8144859860	5.1967292030
H65	2.6069793373	5.0341718692	3.7792748309
H66	1.7627660956	7.3121171778	1.4899124251
H67	1.5440551070	5.5796744029	1.0984643254
H68	0.1946720136	6.6985587455	0.8863738731
H69	0.7629269370	8.5377363588	3.6239963496
H70	-0.9273010966	8.1015182233	3.2301521877
H71	-0.2894925538	7.7666556276	4.8476974198
H72	-6.1894801541	3.1500277390	-1.3085088353
H73	-5.4437038953	1.8108806874	-0.3856832880
H74	-6.4943588723	2.9694705120	0.4453435567
H75	-3.8649963892	3.9148735746	-2.3770738185
H76	-2.4168494494	4.3971915036	-1.4413527862
H77	-2.8768974643	2.6937520346	-1.5222669825
H78	-5.4963661300	5.6962754375	-1.1254358200
H79	-5.6777884377	5.8053250752	0.6512319444
H80	-4.1725731104	6.3379340664	-0.1054146748
C81	-6.6130223110	6.0777619251	5.4329665396
C82	-4.2335435601	7.7114491976	5.5333964266
C83	-4.7697253188	5.8595244689	7.6220608843
C84	-7.1571655440	7.0652450320	4.6071249051
C85	-8.5268677746	7.1221708677	4.3464753233
C86	-9.3922388701	6.1822834502	4.9131257056
C87	-8.8522508218	5.1809132516	5.7358914565
C88	-7.4883388544	5.1283238506	5.9841327970
S89	-11.1585345201	6.1588595425	4.6758090623
C90	-11.4449233766	7.5103948301	3.4893191727
H91	-3.2008142347	7.7664347195	5.8855893245
H92	-4.8559138233	8.4152848078	6.0952513355
H93	-4.2369271577	7.9670965010	4.4728992147
H94	-3.7261751184	5.9168369864	7.9414901760
H95	-5.1680244540	4.8970931186	7.9464197268
H96	-5.3456240521	6.6732884805	8.0742604598
H97	-6.5171815521	7.8127160609	4.1487870996
H98	-8.9025114058	7.9104652504	3.7034828044
H99	-9.5071666345	4.4350616760	6.1793714314
H100	-7.0994928110	4.3270732204	6.6063491611

H101	-10.9121152819	7.3359360879	2.5516144002
H102	-12.5193172381	7.5066448240	3.2925339838
H103	-11.1660760513	8.4810003424	3.9068324426

bond lengths (angstroms):

C1	-P2	:	1.845531	C1	-H42	:	1.095719
C1	-H43	:	1.092144	C1	-H44	:	1.092225
P2	-C3	:	1.844685	P2	-Co4	:	2.185763
P2	-C31	:	1.844751	C3	-H39	:	1.095783
C3	-H40	:	1.092559	C3	-H41	:	1.091948
Co4	-Se5	:	2.424778	Co4	-Se13	:	2.422422
Co4	-Se15	:	2.412834	Co4	-Se19	:	2.418009
Se5	-Co6	:	2.419869	Se5	-Co8	:	2.414181
Co6	-Se7	:	2.416718	Co6	-Se11	:	2.420560
Co6	-Se13	:	2.420929	Co6	-P32	:	2.185124
Se7	-Co8	:	2.426201	Se7	-Co10	:	2.421659
Co8	-Se9	:	2.422671	Co8	-Se15	:	2.420122
Co8	-P27	:	2.185547	Se9	-Co10	:	2.426702
Se9	-Co14	:	2.425036	Co10	-Se11	:	2.409955
Co10	-Se18	:	2.425222	Co10	-P26	:	2.191733
Se11	-Co12	:	2.418608	Co12	-Se13	:	2.421166
Co12	-Se18	:	2.415795	Co12	-Se19	:	2.423935
Co12	-P22	:	2.183346	Co14	-Se15	:	2.423610
Co14	-P16	:	2.186235	Co14	-Se18	:	2.419255
Co14	-Se19	:	2.416713	P16	-C17	:	1.844829
P16	-C20	:	1.845631	P16	-C21	:	1.844614
C17	-H63	:	1.095769	C17	-H64	:	1.092507
C17	-H65	:	1.091937	C20	-H69	:	1.095719
C20	-H70	:	1.091997	C20	-H71	:	1.092193
C21	-H66	:	1.095722	C21	-H67	:	1.092075
C21	-H68	:	1.092491	P22	-C23	:	1.844050
P22	-C24	:	1.844475	P22	-C25	:	1.845283
C23	-H78	:	1.095740	C23	-H79	:	1.092547
C23	-H80	:	1.091966	C24	-H75	:	1.095800
C24	-H76	:	1.092031	C24	-H77	:	1.092522
C25	-H72	:	1.095725	C25	-H73	:	1.092151
C25	-H74	:	1.092248	P26	-C81	:	1.840719
P26	-C82	:	1.845461	P26	-C83	:	1.848393
P27	-C28	:	1.845550	P27	-C29	:	1.844639
P27	-C30	:	1.844441	C28	-H51	:	1.095715
C28	-H52	:	1.092164	C28	-H53	:	1.092230
C29	-H48	:	1.095780	C29	-H49	:	1.091993
C29	-H50	:	1.092570	C30	-H45	:	1.095782
C30	-H46	:	1.092461	C30	-H47	:	1.091980
C31	-H36	:	1.095796	C31	-H37	:	1.092018
C31	-H38	:	1.092491	P32	-C33	:	1.844358
P32	-C34	:	1.844440	P32	-C35	:	1.845755
C33	-H60	:	1.095714	C33	-H61	:	1.091893
C33	-H62	:	1.092570	C34	-H54	:	1.095753
C34	-H55	:	1.092568	C34	-H56	:	1.091977
C35	-H57	:	1.095734	C35	-H58	:	1.092269
C35	-H59	:	1.092158	C81	-C84	:	1.397580

C81	-C88	:	1.404064	C82	-H91	:	1.092517
C82	-H92	:	1.094719	C82	-H93	:	1.090881
C83	-H94	:	1.092848	C83	-H95	:	1.090928
C83	-H96	:	1.094694	C84	-C85	:	1.395444
C84	-H97	:	1.085526	C85	-C86	:	1.397622
C85	-H98	:	1.084415	C86	-C87	:	1.404020
C86	-S89	:	1.782321	C87	-C88	:	1.387316
C87	-H99	:	1.087145	C88	-H100	:	1.086442
S89	-C90	:	1.821105	C90	-H101	:	1.092525
C90	-H102	:	1.092273	C90	-H103	:	1.092771

bond angles:

H42	-C1	-P2	: 110.627381	H43	-C1	-P2	: 109.262378
H43	-C1	-H42	: 109.735481	H44	-C1	-P2	: 109.139382
H44	-C1	-H42	: 109.733833	H44	-C1	-H43	: 108.301313
C3	-P2	-C1	: 101.476073	Co4	-P2	-C1	: 116.130195
Co4	-P2	-C3	: 116.582269	C31	-P2	-C1	: 101.643721
C31	-P2	-C3	: 102.013444	C31	-P2	-Co4	: 116.552449
H39	-C3	-P2	: 110.736142	H40	-C3	-P2	: 109.123434
H40	-C3	-H39	: 109.629134	H41	-C3	-P2	: 109.576907
H41	-C3	-H39	: 109.818306	H41	-C3	-H40	: 107.904308
Se5	-Co4	-P2	: 101.895858	Se13	-Co4	-P2	: 97.370833
Se13	-Co4	-Se5	: 88.803627	Se15	-Co4	-P2	: 101.341882
Se15	-Co4	-Se5	: 87.856211	Se15	-Co4	-Se13	: 161.280254
Se19	-Co4	-P2	: 97.766019	Se19	-Co4	-Se5	: 160.336439
Se19	-Co4	-Se13	: 88.938097	Se19	-Co4	-Se15	: 88.043897
Co6	-Se5	-Co4	: 74.909798	Co8	-Se5	-Co4	: 75.653496
Co8	-Se5	-Co6	: 75.712989	Se7	-Co6	-Se5	: 88.098637
Se11	-Co6	-Se5	: 160.393812	Se11	-Co6	-Se7	: 87.456945
Se13	-Co6	-Se5	: 88.952151	Se13	-Co6	-Se7	: 161.273720
Se13	-Co6	-Se11	: 89.156997	P32	-Co6	-Se5	: 97.996748
P32	-Co6	-Se7	: 101.916513	P32	-Co6	-Se11	: 101.604716
P32	-Co6	-Se13	: 96.806185	Co8	-Se7	-Co6	: 75.549796

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 Co10    -Se7     -Co6     :  75.966790  Co10    -Se7     -Co8     :
75.376691
 Se7     -Co8     -Se5     :  88.011435  Se9     -Co8     -Se5     :
161.201407
 Se9     -Co8     -Se7     :  88.600000  Se15    -Co8     -Se5     :
87.932074
 Se15    -Co8     -Se7     : 160.046700  Se15    -Co8     -Se9     :
88.976874
 P27     -Co8     -Se5     : 101.583759  P27     -Co8     -Se7     :
101.899012
 P27     -Co8     -Se9     :  97.208625  P27     -Co8     -Se15    :
98.054171
 Co10    -Se9     -Co8     :  75.349054  Co14    -Se9     -Co8     :
74.921225
 Co14    -Se9     -Co10    :  74.861807  Se9     -Co10    -Se7     :
88.611752
 Se11    -Co10    -Se7     :  87.585224  Se11    -Co10    -Se9     :
160.698931
 Se18    -Co10    -Se7     : 159.767618  Se18    -Co10    -Se9     :
89.171655
 Se18    -Co10    -Se11    :  87.894894  P26     -Co10    -Se7     :
100.635020
 P26     -Co10    -Se9     :  96.019360  P26     -Co10    -Se11    :
103.279844
 P26     -Co10    -Se18    :  99.597072  Co10    -Se11    -Co6     :
76.112206
 Co12    -Se11    -Co6     :  74.924056  Co12    -Se11    -Co10    :
76.028704
 Se13    -Co12    -Se11    :  89.197013  Se18    -Co12    -Se11    :
87.913159
 Se18    -Co12    -Se13    : 161.228441  Se19    -Co12    -Se11    :
160.069968
 Se19    -Co12    -Se13    :  88.829748  Se19    -Co12    -Se18    :
87.605485
 P22     -Co12    -Se11    :  97.548334  P22     -Co12    -Se13    :
97.350233
 P22     -Co12    -Se18    : 101.415954  P22     -Co12    -Se19    :
102.373468
 Co6     -Se13    -Co4     :  74.933382  Co12    -Se13    -Co4     :
75.014549
 Co12    -Se13    -Co6     :  74.871003  Se15    -Co14    -Se9     :
88.841094
 P16     -Co14    -Se9     :  97.022855  P16     -Co14    -Se15    :
101.176695
 Se18    -Co14    -Se9     :  89.349688  Se18    -Co14    -Se15    :
160.516124
 Se18    -Co14    -P16     :  98.298874  Se19    -Co14    -Se9     :
161.285150
 Se19    -Co14    -Se15    :  87.827135  Se19    -Co14    -P16     :
101.689841
 Se19    -Co14    -Se18    :  87.691148  Co8     -Se15    -Co4     :
75.764233
 Co14    -Se15    -Co4     :  75.592211  Co14    -Se15    -Co8     :
74.993276
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 C17     -P16     -Co14    : 116.453143  C20     -P16     -Co14    :
116.174640
 C20     -P16     -C17     : 101.514879  C21     -P16     -Co14    :
116.654556
 C21     -P16     -C17     : 102.041006  C21     -P16     -C20     :
101.555995
 H63     -C17     -P16     : 110.761738  H64     -C17     -P16     :
109.068396
 H64     -C17     -H63     : 109.622224  H65     -C17     -P16     :
109.518821
 H65     -C17     -H63     : 109.823965  H65     -C17     -H64     :
107.994204
 Co12    -Se18    -Co10    :  75.798391  Co14    -Se18    -Co10    :
74.993231
 Co14    -Se18    -Co12    :  75.782459  Co12    -Se19    -Co4     :
75.044307
 Co14    -Se19    -Co4     :  75.624242  Co14    -Se19    -Co12    :
75.679236
 H69     -C20     -P16     : 110.652594  H70     -C20     -P16     :
109.270773
 H70     -C20     -H69     : 109.764298  H71     -C20     -P16     :
109.103294
 H71     -C20     -H69     : 109.681759  H71     -C20     -H70     :
108.326921
 H66     -C21     -P16     : 110.771218  H67     -C21     -P16     :
109.573295
 H67     -C21     -H66     : 109.762232  H68     -C21     -P16     :
109.166189
 H68     -C21     -H66     : 109.660259  H68     -C21     -H67     :
107.853369
 C23     -P22     -Co12    : 116.410486  C24     -P22     -Co12    :
116.324676
 C24     -P22     -C23     : 102.184748  C25     -P22     -Co12    :
116.275603
 C25     -P22     -C23     : 101.564680  C25     -P22     -C24     :
101.695885
 H78     -C23     -P22     : 110.755741  H79     -C23     -P22     :
109.007336
 H79     -C23     -H78     : 109.698554  H80     -C23     -P22     :
109.540765
 H80     -C23     -H78     : 109.824241  H80     -C23     -H79     :
107.961662
 H75     -C24     -P22     : 110.845809  H76     -C24     -P22     :
109.496201
 H76     -C24     -H75     : 109.833728  H77     -C24     -P22     :
109.084855
 H77     -C24     -H75     : 109.615079  H77     -C24     -H76     :
107.909235
 H72     -C25     -P22     : 110.633674  H73     -C25     -P22     :
109.216221
 H73     -C25     -H72     : 109.722799  H74     -C25     -P22     :
109.153186
 H74     -C25     -H72     : 109.726895  H74     -C25     -H73     :
108.347815
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 C81     -P26     -Co10    : 118.446665  C82     -P26     -Co10    :
115.159793
 C82     -P26     -C81     : 103.161533  C83     -P26     -Co10    :
114.890334
 C83     -P26     -C81     : 102.154265  C83     -P26     -C82     :
100.620386
 C28     -P27     -Co8     : 116.053459  C29     -P27     -Co8     :
116.734631
 C29     -P27     -C28     : 101.545220  C30     -P27     -Co8     :
116.353301
 C30     -P27     -C28     : 101.671082  C30     -P27     -C29     :
102.067203
 H51     -C28     -P27     : 110.645537  H52     -C28     -P27     :
109.189820
 H52     -C28     -H51     : 109.751080  H53     -C28     -P27     :
109.187292
 H53     -C28     -H51     : 109.722369  H53     -C28     -H52     :
108.303210
 H48     -C29     -P27     : 110.762379  H49     -C29     -P27     :
109.552040
 H49     -C29     -H48     : 109.817191  H50     -C29     -P27     :
109.149456
 H50     -C29     -H48     : 109.642203  H50     -C29     -H49     :
107.863348
 H45     -C30     -P27     : 110.782501  H46     -C30     -P27     :
109.087811
 H46     -C30     -H45     : 109.638378  H47     -C30     -P27     :
109.493924
 H47     -C30     -H45     : 109.822688  H47     -C30     -H46     :
107.962811
 H36     -C31     -P2      : 110.738249  H37     -C31     -P2      :
109.530354
 H37     -C31     -H36     : 109.807923  H38     -C31     -P2      :
109.170115
 H38     -C31     -H36     : 109.610512  H38     -C31     -H37     :
107.932020
 C33     -P32     -Co6     : 116.398056  C34     -P32     -Co6     :
116.534271
 C34     -P32     -C33     : 102.205240  C35     -P32     -Co6     :
116.173813
 C35     -P32     -C33     : 101.599274  C35     -P32     -C34     :
101.522271
 H60     -C33     -P32     : 110.785671  H61     -C33     -P32     :
109.556287
 H61     -C33     -H60     : 109.862414  H62     -C33     -P32     :
109.001018
 H62     -C33     -H60     : 109.580815  H62     -C33     -H61     :
108.001931
 H54     -C34     -P32     : 110.800387  H55     -C34     -P32     :
109.106552
 H55     -C34     -H54     : 109.637670  H56     -C34     -P32     :
109.582680
 H56     -C34     -H54     : 109.771408  H56     -C34     -H55     :
107.887547
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 H57     -C35     -P32     : 110.663235  H58     -C35     -P32     :
109.175179
 H58     -C35     -H57     : 109.680747  H59     -C35     -P32     :
109.242323
 H59     -C35     -H57     : 109.749035  H59     -C35     -H58     :
108.288426
 C84     -C81     -P26     : 122.144032  C88     -C81     -P26     :
120.001676
 C88     -C81     -C84     : 117.841135  H91     -C82     -P26     :
107.388071
 H92     -C82     -P26     : 111.113933  H92     -C82     -H91     :
109.852333
 H93     -C82     -P26     : 110.380191  H93     -C82     -H91     :
107.729707
 H93     -C82     -H92     : 110.274044  H94     -C83     -P26     :
107.942578
 H95     -C83     -P26     : 110.128938  H95     -C83     -H94     :
107.938304
 H96     -C83     -P26     : 110.795530  H96     -C83     -H94     :
110.036908
 H96     -C83     -H95     : 109.932890  C85     -C84     -C81     :
121.423649
 H97     -C84     -C81     : 120.429704  H97     -C84     -C85     :
118.146640
 C86     -C85     -C84     : 120.304009  H98     -C85     -C84     :
118.712806
 H98     -C85     -C86     : 120.982177  C87     -C86     -C85     :
118.625726
 S89     -C86     -C85     : 124.642935  S89     -C86     -C87     :
116.730657
 C88     -C87     -C86     : 120.664313  H99     -C87     -C86     :
119.780068
 H99     -C87     -C88     : 119.554743  C87     -C88     -C81     :
121.132879
 H100    -C88     -C81     : 120.026104  H100    -C88     -C87     :
118.836059
 C90     -S89     -C86     : 103.464554  H101    -C90     -S89     :
111.345571
 H102    -C90     -S89     : 105.635574  H102    -C90     -H101    :
108.936693
 H103    -C90     -S89     : 111.723512  H103    -C90     -H101    :
110.200936
 H103    -C90     -H102    : 108.837241

  torsional angles:

 C1      -P2      -C3      -H39     : -50.783004
 C1      -P2      -C3      -H40     :  69.977536
 C1      -P2      -C3      -H41     :-172.075180
 C1      -P2      -Co4     -Se5     : 135.441928
 C1      -P2      -Co4     -Se13    :  45.113310
 C1      -P2      -Co4     -Se15    :-134.371069
 C1      -P2      -Co4     -Se19    : -44.816896
 C1      -P2      -C31     -H36     :  50.793030
 C1      -P2      -C31     -H37     : 172.042933
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C1      -P2     -C31    -H38    : -69.975948
P2      -Co4    -Se5    -Co6    :-138.552855
P2      -Co4    -Se5    -Co8    : 142.683536
P2      -Co4    -Se13   -Co6    : 143.085181
P2      -Co4    -Se13   -Co12   :-138.904900
P2      -Co4    -Se15   -Co8    :-143.097865
P2      -Co4    -Se15   -Co14   : 139.061604
P2      -Co4    -Se19   -Co12   : 138.441509
P2      -Co4    -Se19   -Co14   :-142.851937
C3      -P2     -C1     -H42    :  52.344100
C3      -P2     -C1     -H43    : 173.257989
C3      -P2     -C1     -H44    : -68.488195
C3      -P2     -Co4    -Se5    :-105.002920
C3      -P2     -Co4    -Se13   : 164.668463
C3      -P2     -Co4    -Se15   : -14.815917
C3      -P2     -Co4    -Se19   :  74.738256
C3      -P2     -C31    -H36    : -53.775559
C3      -P2     -C31    -H37    :  67.474345
C3      -P2     -C31    -H38    :-174.544536
Co4     -P2     -C1     -H42    : 179.802205
Co4     -P2     -C1     -H43    : -59.283906
Co4     -P2     -C1     -H44    :  58.969911
Co4     -P2     -C3     -H39    :-177.947210
Co4     -P2     -C3     -H40    : -57.186670
Co4     -P2     -C3     -H41    :  60.760614
Co4     -P2     -C31    -H36    : 178.069572
Co4     -P2     -C31    -H37    : -60.680524
Co4     -P2     -C31    -H38    :  57.300595
Co4     -Se5    -Co6    -Se7    :-120.204537
Co4     -Se5    -Co6    -Se11   : -43.236779
Co4     -Se5    -Co6    -Se13   :  41.300315
Co4     -Se5    -Co6    -P32    : 138.026545
Co4     -Se5    -Co8    -Se7    : 119.072511
Co4     -Se5    -Co8    -Se9    :  39.317953
Co4     -Se5    -Co8    -Se15   : -41.386786
Co4     -Se5    -Co8    -P27    :-139.186715
Co4     -Se13   -Co6    -Se5    : -41.343714
Co4     -Se13   -Co6    -Se7    :  39.604994
Co4     -Se13   -Co6    -Se11   : 119.140571
Co4     -Se13   -Co6    -P32    :-139.272644
Co4     -Se13   -Co12   -Se11   :-119.076458
Co4     -Se13   -Co12   -Se18   : -37.958943
Co4     -Se13   -Co12   -Se19   :  41.090348
Co4     -Se13   -Co12   -P22    : 143.416042
Co4     -Se15   -Co8    -Se5    :  41.612142
Co4     -Se15   -Co8    -Se7    : -36.780270
Co4     -Se15   -Co8    -Se9    :-119.842105
Co4     -Se15   -Co8    -P27    : 143.021848
Co4     -Se15   -Co14   -Se9    : 120.015263
Co4     -Se15   -Co14   -P16    :-143.054688
Co4     -Se15   -Co14   -Se18   :  35.248639
Co4     -Se15   -Co14   -Se19   : -41.565521
Co4     -Se19   -Co12   -Se11   :  43.232441
Co4     -Se19   -Co12   -Se13   : -41.174638
Co4     -Se19   -Co12   -Se18   : 120.391349
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Co4     -Se19    -Co12    -P22     :-138.443325
Co4     -Se19    -Co14    -Se9     : -38.467112
Co4     -Se19    -Co14    -Se15    :  41.449621
Co4     -Se19    -Co14    -P16     : 142.415999
Co4     -Se19    -Co14    -Se18    :-119.584095
Se5     -Co4     -P2      -C31     :  15.676717
Se5     -Co4     -Se13    -Co6     :  41.244278
Se5     -Co4     -Se13    -Co12    : 119.254197
Se5     -Co4     -Se15    -Co8     : -41.392559
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C81     -C88     -C87     -H99     :-179.734059
C82     -P26     -C81     -C84     :  25.662699
C82     -P26     -C81     -C88     :-155.685669
C82     -P26     -C83     -H94     : -67.051875
C82     -P26     -C83     -H95     : 175.336144
C82     -P26     -C83     -H96     :  53.493012
C83     -P26     -C81     -C84     : 129.783993
C83     -P26     -C81     -C88     : -51.564375
C83     -P26     -C82     -H91     :  65.222887
C83     -P26     -C82     -H92     : -54.935458
C83     -P26     -C82     -H93     :-177.599142
C84     -C81     -C88     -C87     :  -1.058377
C84     -C81     -C88     -H100    : 178.122081
C84     -C85     -C86     -C87     :  -0.502804
C84     -C85     -C86     -S89     : 179.186239
C85     -C84     -C81     -C88     :   0.741743
C85     -C86     -C87     -C88     :   0.188629
C85     -C86     -C87     -H99     :-179.469420
C85     -C86     -S89     -C90     :   3.913341
C86     -C85     -C84     -H97     : 179.999119
C86     -C87     -C88     -H100    :-178.582880
C86     -S89     -C90     -H101    :  60.089635
C86     -S89     -C90     -H102    : 178.201087
C86     -S89     -C90     -H103    : -63.606827
C87     -C86     -C85     -H98     : 179.866935
C87     -C86     -S89     -C90     :-176.392268
C88     -C81     -C84     -H97     :-179.226073
C88     -C87     -C86     -S89     :-179.524932
S89     -C86     -C85     -H98     :  -0.444022
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S89     -C86     -C87     -H99     :   0.817019
H97     -C84     -C85     -H98     :  -0.362310
H99     -C87     -C88     -H100    :   1.075934
```

co6se8_pme3_5_3-thiomethylphenyldimethylphosphine

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.............   10540.28475687116
   (E)  Total one-electron terms.....  -27376.33788505094
   (I)  Total two-electron terms.....   12495.20293948768
   (J)    Coulomb.....................   12918.83582217258
   (K)    Exchange+Correlation.......    -423.63288268490
   (L)  Electronic energy............  -14881.13494556326  (E+I)
   (N)  Total energy.................   -4340.85018869210  (A+L)

 SCFE: SCF energy: DFT(b3lyp)     -4340.85018869210 hartrees


 HOMO energy:    -0.15722
 LUMO energy:    -0.05566

  Orbital energies (hartrees):
   -88.86257   -77.09570   -77.09066   -77.09030   -77.09026   -77.09016
   -77.09001   -10.21716   -10.21295   -10.19182   -10.18878   -10.18801
   -10.18679   -10.18094   -10.17590   -10.17400   -10.17316   -10.17295
   -10.17292   -10.17250   -10.17224   -10.17209   -10.17184   -10.17155
   -10.17143   -10.17142   -10.17137   -10.17127   -10.17113   -10.17099
   -10.17063    -7.93860    -6.57260    -6.56789    -6.56753    -6.56750
    -6.56738    -6.56723    -5.90313    -5.89897    -5.89259    -4.73462
    -4.73437    -4.73139    -4.72973    -4.72970    -4.72935    -4.72934
    -4.72933    -4.72930    -4.72922    -4.72918    -4.72907    -4.72904
    -4.72679    -4.72644    -4.72641    -4.72629    -4.72615    -3.70135
    -3.70110    -3.70074    -3.70067    -3.70038    -3.70030    -2.39560
    -2.39535    -2.39516    -2.39506    -2.39474    -2.39459    -2.39233
    -2.39217    -2.39141    -2.39136    -2.39119    -2.39107    -2.39102
    -2.39096    -2.39092    -2.39091    -2.39066    -2.39063    -0.86115
    -0.79920    -0.76651    -0.76376    -0.76325    -0.76313    -0.76288
    -0.76268    -0.73990    -0.72524    -0.69001    -0.68758    -0.68718
    -0.68711    -0.68688    -0.68680    -0.68658    -0.68624    -0.68601
    -0.68585    -0.68533    -0.65200    -0.64363    -0.61583    -0.61461
    -0.61425    -0.61065    -0.59387    -0.59204    -0.59046    -0.58403
    -0.57944    -0.53819    -0.53726    -0.53653    -0.53621    -0.53612
    -0.53529    -0.50626    -0.45935    -0.44658    -0.43897    -0.43890
    -0.43760    -0.43714    -0.43656    -0.43638    -0.43465    -0.42873
    -0.42652    -0.42187    -0.42151    -0.42135    -0.42120    -0.42106
    -0.42093    -0.42080    -0.42048    -0.42040    -0.42036    -0.40364
    -0.39997    -0.39976    -0.39908    -0.39898    -0.39881    -0.39835
    -0.39821    -0.39813    -0.39727    -0.39705    -0.39592    -0.38887
    -0.38280    -0.38123    -0.38061    -0.38041    -0.38022    -0.37952
    -0.37117    -0.36044    -0.33735    -0.33316    -0.33188    -0.33154
    -0.33130    -0.33114    -0.33095    -0.33079    -0.33023    -0.33013
    -0.32964    -0.32915    -0.32667    -0.32492    -0.31823    -0.31617
    -0.31002    -0.30846    -0.30763    -0.29208    -0.28465    -0.28310
    -0.28182    -0.28092    -0.27975    -0.27913    -0.27803    -0.27733
    -0.27679    -0.27645    -0.27566    -0.27517    -0.25356    -0.25285
    -0.25266    -0.24615    -0.23835    -0.23690    -0.23659    -0.23561
    -0.23065    -0.23017    -0.22899    -0.22793    -0.22725    -0.22669
    -0.22607    -0.22548    -0.22033    -0.21491    -0.21468    -0.20668
```

-0.19892	-0.19650	-0.19585	-0.19164	-0.19068	-0.18878
-0.18161	-0.18017	-0.17934	-0.17017	-0.16072	-0.15953
-0.15722	-0.05566	-0.05266	-0.05224	-0.04509	-0.04382
-0.03605	-0.03524	-0.03360	-0.03181	-0.03120	

final geometry:

		angstroms	
atom	x	y	z
C1	-0.8609313948	0.0764761138	0.4231091651
C2	-0.5101812091	0.0617035206	1.7684365037
C3	0.8438801600	0.0151507024	2.1377544372
C4	1.8181299364	-0.0241491911	1.1392604918
C5	1.4639537844	-0.0142622050	-0.2187753919
C6	0.1142430321	0.0394741792	-0.5748650115
P7	1.2924644936	-0.0340505536	3.9276595359
C8	3.0185185178	0.6130575372	3.9524860744
C9	0.3602528943	1.4220250487	4.5806127924
Co10	0.9688552323	-1.9212128012	4.9904909789
Se11	0.6026528682	-1.0386085501	7.2220590239
Co12	-1.0258091539	-2.8165428283	6.9595090129
Se13	-1.4314438655	-2.0778869821	4.6990085995
Co14	-0.6371538351	-4.3469740063	4.4349521845
Se15	1.2332453647	-3.4816259127	3.1653291922
Co16	2.2120959836	-4.6311450472	5.0543937886
Se17	0.5842103949	-6.4084864311	4.7934569226
Co18	0.2118708397	-5.5080828599	7.0098024317
Se19	-2.0302239440	-4.9214708289	6.3315209605
Se20	3.2151919448	-2.5228117287	5.6741001516
Co21	1.8318437736	-3.0952704579	7.5699792497
P22	3.0850103622	-2.3481006580	9.1947625948
C23	4.1619608911	-0.9060165244	8.7894675927
Se24	2.6057286644	-5.3686516736	7.3265387671
Se25	-0.0337288865	-3.9572226880	8.8469531072
P26	3.8562416291	-5.6364678580	4.0239946099
C27	4.5107910995	-7.1627052909	4.8277701733
C28	3.4951722492	-6.2453688707	2.3201209913
C29	5.3950111600	-4.6562033278	3.7554826072
P30	-1.8330360293	-5.0136193459	2.7309826839
C31	-2.5933226189	-3.6908026479	1.6946759219
C32	-3.2807493672	-6.0899806985	3.1142969811
C33	-0.9491630286	-6.0160631513	1.4580223667
P34	-0.1672645235	-7.4208192372	7.9944642122
C35	-0.3982282474	-7.3866530684	9.8241411741
P36	-2.6808259533	-1.7880945268	7.9478929545
C37	-4.2960773090	-2.6766396106	8.0091936979
C38	-3.1755827972	-0.1618693300	7.2289928733
C39	-2.4196327569	-1.3419377715	9.7179479242
C40	-1.6689604300	-8.3372860104	7.4386144605
C41	1.1408060408	-8.7085155150	7.8065002004
C42	4.2944834439	-3.5282663910	9.9338508923
C43	2.1932155864	-1.7341385685	10.6884701737
H44	-0.1898047569	0.0538105875	-1.6157392051
H45	-1.7495455156	-9.3003792437	7.9548874561
H46	-2.5578284290	-7.7351193984	7.6372606732

H47	-1.6058537296	-8.5030669749	6.3604562416
H48	-0.5678666432	-8.3969292972	10.2129984605
H49	0.4900508313	-6.9569673180	10.2926981677
H50	-1.2489543055	-6.7483894967	10.0726305423
H51	0.8471164921	-9.6343511441	8.3136157539
H52	1.2971437345	-8.9056850558	6.7434566434
H53	2.0776987653	-8.3376942811	8.2272885140
H54	-3.9718810736	0.2984735533	7.8244318291
H55	-2.3053181232	0.4979709892	7.2065852576
H56	-3.5197163656	-0.3089210417	6.2032056794
H57	-5.0564356365	-2.0673289272	8.5105334267
H58	-4.6213495843	-2.9078293904	6.9922310118
H59	-4.1704448031	-3.6216193861	8.5424129493
H60	-3.2889508576	-0.8067847514	10.1159597322
H61	-2.2437854558	-2.2489339819	10.2995413831
H62	-1.5320543255	-0.7100926522	9.7964604159
H63	-3.1066739404	-4.1239566204	0.8286119919
H64	-3.3038298858	-3.1218604374	2.2981842739
H65	-1.8128508942	-3.0048624762	1.3568149718
H66	-3.7989234061	-6.3872622948	2.1956615308
H67	-2.9347306087	-6.9801021899	3.6450393031
H68	-3.9699255260	-5.5542872011	3.7705464396
H69	-1.6291676342	-6.2938737597	0.6449227414
H70	-0.1167863997	-5.4326792513	1.0583123536
H71	-0.5449039889	-6.9169469356	1.9246715762
H72	2.8995295818	-1.3413807081	11.4283447585
H73	1.4994751078	-0.9457055636	10.3881726666
H74	1.6135383804	-2.5493963248	11.1259361132
H75	4.8640807772	-3.0482456421	10.7375549257
H76	3.7604276438	-4.3955594505	10.3282802022
H77	4.9776673583	-3.8806663482	9.1578128667
H78	4.7171172407	-0.5754601390	9.6743477466
H79	4.8596313709	-1.1843528965	7.9971024331
H80	3.5371904085	-0.0887680088	8.4216837668
H81	4.3682592308	-6.7565485013	1.8995648089
H82	2.6494483395	-6.9356356480	2.3601330123
H83	3.2194188636	-5.4017858359	1.6839324070
H84	5.2952995352	-7.6186286687	4.2135239246
H85	4.9098173891	-6.9129379000	5.8129381492
H86	3.6921889003	-7.8732811559	4.9641133922
H87	6.1465089947	-5.2512775658	3.2245081999
H88	5.1568003949	-3.7623075094	3.1744921160
H89	5.7934627096	-4.3331541757	4.7196286302
H90	3.2931773426	0.7844887728	4.9958493738
H91	3.0989181256	1.5472469015	3.3878832497
H92	3.7101791227	-0.1301119861	3.5523198962
H93	0.6805866070	1.6064131355	5.6081414645
H94	-0.7074745324	1.1966099959	4.5964385616
H95	0.5422602628	2.3074084461	3.9633741310
H96	2.8697052194	-0.0796929453	1.4027464961
S97	2.8138989490	-0.0577607547	-1.3885767358
H98	-1.9097993639	0.1167056890	0.1396361782
H99	-1.2849600871	0.0583485527	2.5273806749
C100	1.9777679232	-0.2454030075	-2.9957649497
H101	2.7775110806	-0.3434181006	-3.7333664769

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 H102          1.3614237656     -1.1474302991     -3.0199204429
 H103          1.3739238207      0.6303943295     -3.2457492198


 bond lengths (angstroms):

C1      -C2      :   1.390377      C1      -C6      :   1.395810
C1      -H98     :   1.087244      C2      -C3      :   1.404295
C2      -H99     :   1.084569      C3      -C4      :   1.395599
C3      -P7      :   1.845917      C4      -C5      :   1.403496
C4      -H96     :   1.085505      C5      -C6      :   1.396928
C5      -S97     :   1.786807      C6      -H44     :   1.084467
P7      -C8      :   1.843537      P7      -C9      :   1.848113
P7      -Co10    :   2.189912      C8      -H90     :   1.092444
C8      -H91     :   1.094509      C8      -H92     :   1.091251
C9      -H93     :   1.091983      C9      -H94     :   1.091377
C9      -H95     :   1.094538      Co10    -Se11    :   2.427548
Co10    -Se13    :   2.423003      Co10    -Se15    :   2.415783
Co10    -Se20    :   2.423896      Se11    -Co12    :   2.425257
Se11    -Co21    :   2.421119      Co12    -Se13    :   2.412471
Co12    -Se19    :   2.415355      Co12    -Se25    :   2.418226
Co12    -P36     :   2.184877      Se13    -Co14    :   2.418549
Co14    -Se15    :   2.420571      Co14    -Se17    :   2.422827
Co14    -Se19    :   2.422326      Co14    -P30     :   2.185878
Se15    -Co16    :   2.418286      Co16    -Se17    :   2.424261
Co16    -Se20    :   2.415638      Co16    -Se24    :   2.421055
Co16    -P26     :   2.185317      Se17    -Co18    :   2.421064
Co18    -Se19    :   2.414781      Co18    -Se24    :   2.418743
Co18    -Se25    :   2.416735      Co18    -P34     :   2.184459
Se20    -Co21    :   2.415723      Co21    -P22     :   2.183715
Co21    -Se24    :   2.413799      Co21    -Se25    :   2.419501
P22     -C23     :   1.844910      P22     -C42     :   1.844415
P22     -C43     :   1.844833      C23     -H78     :   1.095664
C23     -H79     :   1.091814      C23     -H80     :   1.092473
P26     -C27     :   1.844964      P26     -C28     :   1.845079
P26     -C29     :   1.844134      C27     -H84     :   1.095727
C27     -H85     :   1.091862      C27     -H86     :   1.092528
C28     -H81     :   1.095652      C28     -H82     :   1.092391
C28     -H83     :   1.091974      C29     -H87     :   1.095808
C29     -H88     :   1.092403      C29     -H89     :   1.092109
P30     -C31     :   1.844400      P30     -C32     :   1.844277
P30     -C33     :   1.845685      C31     -H63     :   1.096001
C31     -H64     :   1.092126      C31     -H65     :   1.092612
C32     -H66     :   1.095797      C32     -H67     :   1.092581
C32     -H68     :   1.092060      C33     -H69     :   1.095772
C33     -H70     :   1.092225      C33     -H71     :   1.092144
P34     -C35     :   1.844513      P34     -C40     :   1.844985
P34     -C41     :   1.845140      C35     -H48     :   1.095740
C35     -H49     :   1.092344      C35     -H50     :   1.092182
P36     -C37     :   1.844534      P36     -C38     :   1.845592
P36     -C39     :   1.844010      C37     -H57     :   1.095785
C37     -H58     :   1.092458      C37     -H59     :   1.092288
C38     -H54     :   1.095698      C38     -H55     :   1.092361
C38     -H56     :   1.091921      C39     -H60     :   1.095681
C39     -H61     :   1.091703      C39     -H62     :   1.092331
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 C40     -H45     :   1.095710      C40     -H46     :   1.091857
 C40     -H47     :   1.092653      C41     -H51     :   1.095715
 C41     -H52     :   1.092419      C41     -H53     :   1.091943
 C42     -H75     :   1.095811      C42     -H76     :   1.092240
 C42     -H77     :   1.092319      C43     -H72     :   1.095697
 C43     -H73     :   1.092282      C43     -H74     :   1.091809
 S97     -C100    :   1.821367      C100    -H101    :   1.092361
 C100    -H102    :   1.092757      C100    -H103    :   1.092768

  bond angles:

 C6      -C1      -C2      : 121.016416  H98     -C1      -C2      :
119.738151
 H98     -C1      -C6      : 119.245418  C3      -C2      -C1      :
119.872278
 H99     -C2      -C1      : 119.795932  H99     -C2      -C3      :
120.309889
 C4      -C3      -C2      : 119.070744  P7      -C3      -C2      :
119.354813
 P7      -C3      -C4      : 121.557473  C5      -C4      -C3      :
121.059123
 H96     -C4      -C3      : 120.267889  H96     -C4      -C5      :
118.665467
 C6      -C5      -C4      : 119.389677  S97     -C5      -C4      :
116.273512
 S97     -C5      -C6      : 124.334333  C5      -C6      -C1      :
119.590299
 H44     -C6      -C1      : 119.341323  H44     -C6      -C5      :
121.068358
 C8      -P7      -C3      : 103.369500  C9      -P7      -C3      :
101.478949
 C9      -P7      -C8      : 101.008568  Co10    -P7      -C3      :
117.236364
 Co10    -P7      -C8      : 115.741230  Co10    -P7      -C9      :
115.654319
 H90     -C8      -P7      : 107.658292  H91     -C8      -P7      :
111.187940
 H91     -C8      -H90     : 109.893166  H92     -C8      -P7      :
110.453312
 H92     -C8      -H90     : 107.322200  H92     -C8      -H91     :
110.215245
 H93     -C9      -P7      : 108.513083  H94     -C9      -P7      :
109.625874
 H94     -C9      -H93     : 107.952267  H95     -C9      -P7      :
110.744458
 H95     -C9      -H93     : 110.198298  H95     -C9      -H94     :
109.751094
 Se11    -Co10    -P7      :  98.924123  Se13    -Co10    -P7      :
98.263493
 Se13    -Co10    -Se11    :  89.120835  Se15    -Co10    -P7      :
100.007635
 Se15    -Co10    -Se11    : 161.062921  Se15    -Co10    -Se13    :
88.611250
 Se20    -Co10    -P7      : 102.345853  Se20    -Co10    -Se11    :
88.325592
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 Se20    -Co10    -Se13    : 159.380784  Se20    -Co10    -Se15    :
87.210680
 Co12    -Se11    -Co10    :  74.647223  Co21    -Se11    -Co10    :
75.325085
 Co21    -Se11    -Co12    :  74.556771  Se13    -Co12    -Se11    :
89.420003
 Se19    -Co12    -Se11    : 161.127826  Se19    -Co12    -Se13    :
87.322765
 Se25    -Co12    -Se11    :  89.188530  Se25    -Co12    -Se13    :
160.864697
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Co14    -P30     -C31     -H64     : -63.194480
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Co14    -P30     -C33     -H70     : -58.823073
Co14    -P30     -C33     -H71     :  59.495399
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Se15    -Co10    -Se20    -Co16    : -41.701791
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Se15    -Co14    -Se17    -Co18    : 118.710770
Se15    -Co14    -Se19    -Co18    : -42.800700
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Se15    -Co14    -P30     -C32     : 168.112770
Se15    -Co14    -P30     -C33     :  48.348961
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Se15    -Co16    -Se20    -Co21    : 119.875200
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Se15    -Co16    -P26     -C27     :-155.862521
Se15    -Co16    -P26     -C28     : -36.638663
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Co16    -Se15    -Co14    -Se17    : -41.104638
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Se17    -Co18    -P34     -C40     : -64.398363
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Co18    -Se24    -Co16    -Se20    : 120.142755
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Co18    -P34     -C40     -H47     :  56.754905
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Co21    -Se20    -Co16    -Se24    : -41.487850
Co21    -Se20    -Co16    -P26     :-141.578367
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Co21    -P22     -C23     -H79     : -61.305090
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Co21    -P22     -C42     -H75     :-179.852445
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Co21    -Se24    -Co18    -Se25    : -41.689320
Co21    -Se24    -Co18    -P34     :-143.139723
Co21    -Se25    -Co12    -P36     :-137.759956
Co21    -Se25    -Co18    -Se24    :  41.584705
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C23     -P22     -Co21    -Se24    : 119.573631
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C23     -P22     -C42     -H76     : 173.514068
C23     -P22     -C42     -H77     : -68.579886
C23     -P22     -C43     -H72     : -50.806318
C23     -P22     -C43     -H73     :  69.881624
C23     -P22     -C43     -H74     :-172.035960
Se24    -Co16    -P26     -C27     :  25.232887
Se24    -Co16    -P26     -C28     : 144.456745
Se24    -Co16    -P26     -C29     : -95.332099
Se24    -Co18    -P34     -C35     :  84.722384
Se24    -Co18    -P34     -C40     :-154.846385
Se24    -Co18    -P34     -C41     : -35.523122
Se24    -Co21    -P22     -C42     :  -0.877100
Se24    -Co21    -P22     -C43     :-121.330498
Se25    -Co12    -P36     -C37     : -91.627568
Se25    -Co12    -P36     -C38     : 148.219889
Se25    -Co12    -P36     -C39     :  28.981367
Se25    -Co18    -P34     -C35     :  -5.096556
Se25    -Co18    -P34     -C40     : 115.334676
Se25    -Co18    -P34     -C41     :-125.342062
Se25    -Co21    -P22     -C42     :  89.213944
Se25    -Co21    -P22     -C43     : -31.239455
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C27     -P26     -C28     -H83     :-172.506298
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C27     -P26     -C29     -H89     : -68.481443
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C41     -P34     -C40     -H46     : 171.666764
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C42     -P22     -C23     -H80     :-174.843580
C42     -P22     -C43     -H72     :  54.087917
C42     -P22     -C43     -H73     : 174.775860
C42     -P22     -C43     -H74     : -67.141725
C43     -P22     -C23     -H78     :  50.714820
C43     -P22     -C23     -H79     : 171.951906
C43     -P22     -C23     -H80     : -69.944977
C43     -P22     -C42     -H75     : -52.175411
C43     -P22     -C42     -H76     :  68.871338
C43     -P22     -C42     -H77     :-173.222616
H44     -C6      -C1      -H98     :   0.143522
H44     -C6      -C5      -S97     :   0.260089
H96     -C4      -C5      -S97     :  -1.367134
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H98 -C1 -C2 -H99 : 1.950039

co6se8_pme3_5_monoenedimethylphosphine

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.............   11924.65668770505
   (E)  Total one-electron terms.....  -30553.49547246084
   (I)  Total two-electron terms.....   13979.52870105361
   (J)    Coulomb.....................   14448.86835300831
   (K)    Exchange+Correlation.......    -469.33965195470
   (L)  Electronic energy............  -16573.96677140723  (E+I)
   (N)  Total energy.................   -4649.31008370219  (A+L)

 SCFE: SCF energy: DFT(b3lyp)     -4649.31008370219 hartrees


 HOMO energy:    -0.15740
 LUMO energy:    -0.06040

  Orbital energies (hartrees):
   -88.86743   -77.09494   -77.09073   -77.09062   -77.09050   -77.09043
   -77.09018   -10.21968   -10.21651   -10.19402   -10.19397   -10.19118
   -10.18936   -10.18916   -10.18823   -10.18758   -10.18718   -10.18573
   -10.18554   -10.18455   -10.18317   -10.18270   -10.17498   -10.17374
   -10.17326   -10.17300   -10.17290   -10.17281   -10.17280   -10.17277
   -10.17243   -10.17229   -10.17216   -10.17174   -10.17168   -10.17126
   -10.17116   -10.17101   -10.17055    -7.94332    -6.57186    -6.56799
    -6.56787    -6.56771    -6.56765    -6.56739    -5.90781    -5.90369
    -5.89741    -4.73385    -4.73363    -4.73066    -4.72981    -4.72980
    -4.72970    -4.72967    -4.72955    -4.72951    -4.72948    -4.72946
    -4.72923    -4.72920    -4.72689    -4.72677    -4.72661    -4.72656
    -4.72631    -3.70133    -3.70125    -3.70101    -3.70066    -3.70060
    -3.70040    -2.39597    -2.39532    -2.39532    -2.39508    -2.39501
    -2.39484    -2.39211    -2.39194    -2.39183    -2.39176    -2.39165
    -2.39142    -2.39113    -2.39105    -2.39100    -2.39093    -2.39054
    -2.39023    -0.86636    -0.85557    -0.81346    -0.78928    -0.76388
    -0.76351    -0.76337    -0.76314    -0.76300    -0.76278    -0.74887
    -0.74296    -0.73996    -0.70699    -0.68920    -0.68766    -0.68753
    -0.68745    -0.68721    -0.68707    -0.68676    -0.68646    -0.68623
    -0.68604    -0.68557    -0.65804    -0.64357    -0.62538    -0.61498
    -0.61448    -0.61393    -0.61030    -0.60135    -0.59421    -0.59120
    -0.59101    -0.58140    -0.57967    -0.55597    -0.54797    -0.53749
    -0.53696    -0.53659    -0.53630    -0.53554    -0.50554    -0.49517
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    -0.43801    -0.43767    -0.43693    -0.43682    -0.43662    -0.43086
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    -0.42129    -0.42121    -0.42088    -0.42074    -0.42055    -0.42039
    -0.41655    -0.40360    -0.40122    -0.39993    -0.39951    -0.39923
    -0.39905    -0.39899    -0.39841    -0.39796    -0.39755    -0.39745
    -0.39634    -0.39208    -0.38950    -0.38107    -0.38098    -0.38078
    -0.38069    -0.38039    -0.38015    -0.37154    -0.36816    -0.35647
    -0.34676    -0.33923    -0.33382    -0.33201    -0.33174    -0.33167
    -0.33150    -0.33128    -0.33106    -0.33058    -0.33049    -0.33010
    -0.32978    -0.32775    -0.32676    -0.32593    -0.32072    -0.31790
    -0.31590    -0.30933    -0.30890    -0.30754    -0.28945    -0.28508
    -0.28265    -0.28243    -0.28123    -0.27989    -0.27901    -0.27796
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-0.27779	-0.27749	-0.27563	-0.27495	-0.26973	-0.25501
-0.25365	-0.25291	-0.25251	-0.24795	-0.23813	-0.23739
-0.23684	-0.23551	-0.23208	-0.23045	-0.22964	-0.22907
-0.22779	-0.22757	-0.22666	-0.22578	-0.22553	-0.22060
-0.21497	-0.21487	-0.19906	-0.19644	-0.19594	-0.19229
-0.19164	-0.18986	-0.18922	-0.18141	-0.18011	-0.17929
-0.16983	-0.16057	-0.15986	-0.15740	-0.06040	-0.05282
-0.05237	-0.04813	-0.04408	-0.04192	-0.03577	-0.03538
-0.03385	-0.03174				

final geometry:

		angstroms	
atom	x	y	z
C1	-0.4483028530	0.3610629003	0.0431764832
C2	-0.3970962806	0.4153668453	1.4464258215
C3	0.8595532595	0.4643185467	2.0588687470
C4	2.0218912251	0.4217150402	1.2954089269
C5	1.9805046282	0.3251950924	-0.1053709313
C6	0.7105016514	0.3269910788	-0.7163307336
P7	-1.9507359051	0.2629156200	2.4123213660
C8	-3.0103633509	1.5960961606	1.6956526523
C9	3.2378149219	0.1685099105	-0.8348802647
Co10	-2.8509232275	-1.7363869544	2.4758400181
Se11	-1.7732060973	-2.6182787495	4.4604676688
Co12	-4.0927933810	-3.2870705462	4.6457842610
Se13	-3.3259070728	-5.5781919271	4.6929151838
Co14	-1.9588383285	-4.5262295253	2.9888043108
P15	-0.0093217482	-5.4741886857	3.2594064266
C16	0.8270776826	-6.0727287679	1.7267718224
Co17	-3.5027464642	-3.9173855316	0.5544730832
P18	-3.2176894175	-4.3394888942	-1.5705907160
C19	-3.9872600649	-5.8931750332	-2.2026703394
Co20	-4.7405353113	-5.4577362672	2.7350760261
Se21	-6.2822779233	-4.1262974814	4.0309334613
Co22	-5.6346275890	-2.6767690620	2.2046741991
P23	-7.5576957489	-1.6893645441	1.8873506736
C24	-7.5161447436	-0.1038169173	0.9448679384
P25	-5.6355604009	-7.4438515633	2.8978225365
C26	-6.4956813871	-8.0786589490	1.3947933054
C27	-4.4819943183	-8.8327709684	3.2796741113
C28	-6.9219232461	-7.6628053191	4.2010831000
Se29	-5.8195983912	-4.5892405805	0.7434536459
Se30	-2.8450461137	-6.0994479105	1.3742968263
Se31	-4.2595842492	-1.6227517761	0.5119050220
Se32	-1.3246326248	-3.0732271678	1.1691704070
Se33	-4.7599940647	-1.1019775040	3.8258304256
P34	-4.3545615583	-2.8692066768	6.7738046858
C35	-3.6451959818	-4.0990099799	7.9511732144
C36	-6.0935683102	-2.7210467159	7.3702010500
C37	-3.6135502262	-1.2958325108	7.3908866669
C38	1.3118687247	-4.4332114440	4.0159378674
C39	0.0274926107	-6.9833416360	4.3195662179
C40	-1.5252291038	0.9972891386	4.0492672591
C41	-8.4719877499	-1.1933474917	3.4113345782

C42	-8.8445028454	-2.6450487845	0.9744324698
C43	-1.4735786305	-4.5325947116	-2.1400807295
C44	-3.8747032235	-3.0923908930	-2.7610065537
H45	-6.8787057374	-9.0912269689	1.5640462388
H46	-7.3189924474	-7.4099615820	1.1352056723
H47	-5.7934649618	-8.0877593470	0.5578799554
H48	-7.2827774604	-8.6971881928	4.2212943900
H49	-6.4939594994	-7.4043424336	5.1725654356
H50	-7.7555109301	-6.9838270638	4.0097596574
H51	-5.0284549239	-9.7799809782	3.3490622022
H52	-3.7271299651	-8.8995629619	2.4932112435
H53	-3.9751326008	-8.6290465905	4.2254610786
H54	-8.5172503815	0.3369960295	0.8795055966
H55	-6.8406391089	0.5928049093	1.4468455075
H56	-7.1262180750	-0.2865525802	-0.0586827409
H57	-9.7761366748	-2.0723977216	0.9042547246
H58	-8.4810713913	-2.8830249793	-0.0275999058
H59	-9.0302618431	-3.5866490083	1.4964495805
H60	-9.4160106000	-0.7007137041	3.1532358328
H61	-8.6719071383	-2.0808949258	4.0155355373
H62	-7.8492603010	-0.5132591695	3.9967310459
H63	-3.7060115902	-3.4156961749	-3.7944238210
H64	-4.9453241758	-2.9598153812	-2.5881275538
H65	-3.3859251313	-2.1308138655	-2.5903886153
H66	-3.7804426726	-6.0199621525	-3.2712527571
H67	-3.5865795331	-6.7438396420	-1.6469080747
H68	-5.0661630090	-5.8529038240	-2.0378136738
H69	-1.4383915338	-4.7763090716	-3.2078591671
H70	-0.9229232004	-3.6085841063	-1.9522827952
H71	-0.9971768723	-5.3311000023	-1.5663703346
H72	-6.1192882150	-2.4707688920	8.4366918223
H73	-6.6021383412	-1.9418201188	6.7977058750
H74	-6.6188782819	-3.6627085687	7.1977720316
H75	-3.8033764859	-3.7812510429	8.9878861694
H76	-4.1117866550	-5.0725922960	7.7871099442
H77	-2.5748984735	-4.2035805923	7.7580625633
H78	-3.8031884962	-1.1734210410	8.4631000371
H79	-2.5373342718	-1.3092128715	7.2056052969
H80	-4.0460983835	-0.4562931569	6.8422283641
H81	1.7960254009	-6.5241554062	1.9674350790
H82	0.1903884655	-6.8092712648	1.2319028015
H83	0.9726872161	-5.2310853378	1.0459518129
H84	1.0391833774	-7.4016813478	4.3674556425
H85	-0.3164583789	-6.7312039120	5.3249835139
H86	-0.6576103331	-7.7274031642	3.9064316950
H87	2.2584100187	-4.9832152160	4.0652740972
H88	1.4417502603	-3.5306943436	3.4138481310
H89	1.0078122433	-4.1286498879	5.0195328274
H90	-2.4517061481	1.0812887452	4.6222363744
H91	-1.0709461533	1.9862123974	3.9316168205
H92	-0.8536572315	0.3349977197	4.5973507198
H93	-3.9330232393	1.6477119407	2.2791703027
H94	-3.2756121331	1.3513225481	0.6662437515
H95	-2.4929894442	2.5603590409	1.7280844847
H96	0.9447125481	0.5099522495	3.1401537860

H97	2.9883879003	0.4419201640	1.7947272576
H98	0.6272875737	0.2708336113	-1.7981180733
H99	-1.4097885237	0.3062647281	-0.4600346531
C100	3.3910335074	-0.0283413228	-2.1598522166
H101	4.1256145259	0.1747307349	-0.2039677841
C102	4.6407997418	-0.2909525291	-2.8698047490
H103	2.5051423904	-0.0356760491	-2.7929547335
C104	4.6106126235	-0.4701603458	-4.2663271739
C105	5.7559868972	-0.7616139772	-4.9924607417
C106	6.9943977212	-0.8843700594	-4.3447014990
C107	7.0450471104	-0.7081663361	-2.9553951354
C108	5.8910166279	-0.4149604539	-2.2381571997
H109	3.6600105399	-0.3873178482	-4.7885628250
H110	5.6933532280	-0.8980030707	-6.0690696230
S111	8.3985271786	-1.2856449798	-5.3660726516
H112	7.9836537058	-0.8007665229	-2.4202260161
H113	5.9690546589	-0.2976013724	-1.1608993144
C114	9.7695659881	-1.4040855812	-4.1728557189
H115	10.6555456722	-1.6482353695	-4.7634515015
H116	9.9362489804	-0.4541297004	-3.6578964366
H117	9.6001060211	-2.2020447436	-3.4460859758

bond lengths (angstroms):

C1	-C2	:	1.405233	C1	-C6	:	1.385944
C1	-H99	:	1.086591	C2	-C3	:	1.398803
C2	-P7	:	1.835754	C3	-C4	:	1.391300
C3	-H96	:	1.085593	C4	-C5	:	1.404711
C4	-H97	:	1.088045	C5	-C6	:	1.409320
C5	-C9	:	1.462041	C6	-H98	:	1.086435
P7	-C8	:	1.847646	P7	-Co10	:	2.193532
P7	-C40	:	1.843896	C8	-H93	:	1.092913
C8	-H94	:	1.090850	C8	-H95	:	1.094774
C9	-C100	:	1.348250	C9	-H101	:	1.089164
Co10	-Se11	:	2.424449	Co10	-Se31	:	2.419562
Co10	-Se32	:	2.413315	Co10	-Se33	:	2.422705
Se11	-Co12	:	2.421179	Se11	-Co14	:	2.416719
Co12	-Se13	:	2.416521	Co12	-Se21	:	2.424085
Co12	-Se33	:	2.427367	Co12	-P34	:	2.184400
Se13	-Co14	:	2.424767	Se13	-Co20	:	2.418433
Co14	-P15	:	2.184598	Co14	-Se30	:	2.422192
Co14	-Se32	:	2.413400	P15	-C16	:	1.845747
P15	-C38	:	1.844320	P15	-C39	:	1.844678
C16	-H81	:	1.095703	C16	-H82	:	1.092137
C16	-H83	:	1.092283	Co17	-P18	:	2.185252
Co17	-Se29	:	2.419691	Co17	-Se30	:	2.421999
Co17	-Se31	:	2.416601	Co17	-Se32	:	2.415499
P18	-C19	:	1.845455	P18	-C43	:	1.844866
P18	-C44	:	1.844996	C19	-H66	:	1.095772
C19	-H67	:	1.092267	C19	-H68	:	1.092168
Co20	-Se21	:	2.414321	Co20	-P25	:	2.184539
Co20	-Se29	:	2.425948	Co20	-Se30	:	2.419999
Se21	-Co22	:	2.419877	Co22	-P23	:	2.184915
Co22	-Se29	:	2.413903	Co22	-Se31	:	2.422223

Co22	-Se33	:	2.423448	P23	-C24	:	1.844983
P23	-C41	:	1.845126	P23	-C42	:	1.844620
C24	-H54	:	1.095811	C24	-H55	:	1.092507
C24	-H56	:	1.092039	P25	-C26	:	1.844420
P25	-C27	:	1.845433	P25	-C28	:	1.844223
C26	-H45	:	1.095741	C26	-H46	:	1.091963
C26	-H47	:	1.092527	C27	-H51	:	1.095738
C27	-H52	:	1.092156	C27	-H53	:	1.092211
C28	-H48	:	1.095706	C28	-H49	:	1.092581
C28	-H50	:	1.092009	P34	-C35	:	1.844400
P34	-C36	:	1.844393	P34	-C37	:	1.845371
C35	-H75	:	1.095794	C35	-H76	:	1.092010
C35	-H77	:	1.092595	C36	-H72	:	1.095766
C36	-H73	:	1.092515	C36	-H74	:	1.091975
C37	-H78	:	1.095714	C37	-H79	:	1.092130
C37	-H80	:	1.092223	C38	-H87	:	1.095846
C38	-H88	:	1.092666	C38	-H89	:	1.091976
C39	-H84	:	1.095819	C39	-H85	:	1.092126
C39	-H86	:	1.092554	C40	-H90	:	1.092570
C40	-H91	:	1.094616	C40	-H92	:	1.090887
C41	-H60	:	1.095665	C41	-H61	:	1.092139
C41	-H62	:	1.092245	C42	-H57	:	1.095808
C42	-H58	:	1.092146	C42	-H59	:	1.092529
C43	-H69	:	1.095804	C43	-H70	:	1.091918
C43	-H71	:	1.092572	C44	-H63	:	1.095872
C44	-H64	:	1.092562	C44	-H65	:	1.092083
C100	-C102	:	1.461134	C100	-H103	:	1.088887
C102	-C104	:	1.408297	C102	-C108	:	1.406200
C104	-C105	:	1.387118	C104	-H109	:	1.087767
C105	-C106	:	1.402969	C105	-H110	:	1.087020
C106	-C107	:	1.401351	C106	-S111	:	1.782077
C107	-C108	:	1.390031	C107	-H112	:	1.084418
C108	-H113	:	1.086438	S111	-C114	:	1.821412
C114	-H115	:	1.092416	C114	-H116	:	1.093335
C114	-H117	:	1.092543				

bond angles:

C6	-C1	-C2	: 121.179159	H99	-C1	-C2	: 119.778593
H99	-C1	-C6	: 119.000596	C3	-C2	-C1	: 118.119008
P7	-C2	-C1	: 119.430379	P7	-C2	-C3	: 122.198328
C4	-C3	-C2	: 120.610841	H96	-C3	-C2	: 120.533371
H96	-C3	-C4	: 118.836556	C5	-C4	-C3	: 121.647559
H97	-C4	-C3	: 119.321683	H97	-C4	-C5	: 119.017461
C6	-C5	-C4	: 117.307336	C9	-C5	-C4	: 118.659070
C9	-C5	-C6	: 123.971855	C5	-C6	-C1	: 121.059085

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 H98     -C6      -C1      : 118.874488  H98     -C6      -C5      :
120.040722
 C8      -P7      -C2      : 102.788808  Co10    -P7      -C2      :
115.991912
 Co10    -P7      -C8      : 115.692564  C40     -P7      -C2      :
103.811455
 C40     -P7      -C8      : 100.912865  C40     -P7      -Co10    :
115.594671
 H93     -C8      -P7      : 108.128250  H94     -C8      -P7      :
110.095006
 H94     -C8      -H93     : 108.008427  H95     -C8      -P7      :
110.672057
 H95     -C8      -H93     : 109.971457  H95     -C8      -H94     :
109.907733
 C100    -C9      -C5      : 127.137373  H101    -C9      -C5      :
114.288638
 H101    -C9      -C100    : 118.519885  Se11    -Co10    -P7      :
99.951895
 Se31    -Co10    -P7      :  99.939750  Se31    -Co10    -Se11    :
160.105824
 Se32    -Co10    -P7      : 103.277670  Se32    -Co10    -Se11    :
87.741203
 Se32    -Co10    -Se31    :  87.405952  Se33    -Co10    -P7      :
95.787569
 Se33    -Co10    -Se11    :  89.392185  Se33    -Co10    -Se31    :
88.924457
 Se33    -Co10    -Se32    : 160.930299  Co12    -Se11    -Co10    :
74.767479
 Co14    -Se11    -Co10    :  75.791438  Co14    -Se11    -Co12    :
75.814959
 Se13    -Co12    -Se11    :  87.670225  Se21    -Co12    -Se11    :
160.311606
 Se21    -Co12    -Se13    :  87.899479  Se33    -Co12    -Se11    :
89.359544
 Se33    -Co12    -Se13    : 161.315077  Se33    -Co12    -Se21    :
88.722495
 P34     -Co12    -Se11    :  97.847151  P34     -Co12    -Se13    :
101.560202
 P34     -Co12    -Se21    : 101.834478  P34     -Co12    -Se33    :
97.119361
 Co14    -Se13    -Co12    :  75.752338  Co20    -Se13    -Co12    :
75.602828
 Co20    -Se13    -Co14    :  74.884194  Se13    -Co14    -Se11    :
87.584122
 P15     -Co14    -Se11    : 101.455224  P15     -Co14    -Se13    :
103.168484
 Se30    -Co14    -Se11    : 161.220940  Se30    -Co14    -Se13    :
88.876364
 Se30    -Co14    -P15     :  97.309332  Se32    -Co14    -Se11    :
87.915997
 Se32    -Co14    -Se13    : 159.924161  Se32    -Co14    -P15     :
96.899898
 Se32    -Co14    -Se30    :  89.118978  C16     -P15     -Co14    :
116.247287
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 C38     -P15     -Co14    : 116.433648  C38     -P15     -C16     :
101.479934
 C39     -P15     -Co14    : 116.359388  C39     -P15     -C16     :
101.705250
 C39     -P15     -C38     : 102.223201  H81     -C16     -P15     :
110.606485
 H82     -C16     -P15     : 109.315757  H82     -C16     -H81     :
109.706757
 H83     -C16     -P15     : 109.153600  H83     -C16     -H81     :
109.662334
 H83     -C16     -H82     : 108.357112  Se29    -Co17    -P18     :
98.465778
 Se30    -Co17    -P18     :  96.875949  Se30    -Co17    -Se29    :
89.050001
 Se31    -Co17    -P18     : 101.954502  Se31    -Co17    -Se29    :
88.002912
 Se31    -Co17    -Se30    : 161.168531  Se32    -Co17    -P18     :
101.382033
 Se32    -Co17    -Se29    : 160.145931  Se32    -Co17    -Se30    :
89.074627
 Se32    -Co17    -Se31    :  87.423663  C19     -P18     -Co17    :
116.186645
 C43     -P18     -Co17    : 116.341926  C43     -P18     -C19     :
101.559359
 C44     -P18     -Co17    : 116.771020  C44     -P18     -C19     :
101.512423
 C44     -P18     -C43     : 102.019156  H66     -C19     -P18     :
110.653354
 H67     -C19     -P18     : 109.173566  H67     -C19     -H66     :
109.684525
 H68     -C19     -P18     : 109.220304  H68     -C19     -H66     :
109.749846
 H68     -C19     -H67     : 108.318099  Se21    -Co20    -Se13    :
88.079189
 P25     -Co20    -Se13    :  97.704235  P25     -Co20    -Se21    :
101.523219
 Se29    -Co20    -Se13    : 160.496943  Se29    -Co20    -Se21    :
87.660103
 Se29    -Co20    -P25     : 101.794821  Se30    -Co20    -Se13    :
89.074594
 Se30    -Co20    -Se21    : 161.481638  Se30    -Co20    -P25     :
96.991122
 Se30    -Co20    -Se29    :  88.950973  Co20    -Se21    -Co12    :
75.539132
 Co22    -Se21    -Co12    :  75.066754  Co22    -Se21    -Co20    :
75.780282
 P23     -Co22    -Se21    :  98.322630  Se29    -Co22    -Se21    :
87.808107
 Se29    -Co22    -P23     : 101.693973  Se31    -Co22    -Se21    :
160.052046
 Se31    -Co22    -P23     : 101.624649  Se31    -Co22    -Se29    :
88.006565
 Se33    -Co22    -Se21    :  88.910677  Se33    -Co22    -P23     :
96.958063
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 Se33    -Co22    -Se29    : 161.338003  Se33    -Co22    -Se31    :
88.845509
 C24     -P23     -Co22    : 116.278847  C41     -P23     -Co22    :
115.954959
 C41     -P23     -C24     : 101.657479  C42     -P23     -Co22    :
116.855313
 C42     -P23     -C24     : 102.013029  C42     -P23     -C41     :
101.675809
 H54     -C24     -P23     : 110.830251  H55     -C24     -P23     :
109.097924
 H55     -C24     -H54     : 109.619657  H56     -C24     -P23     :
109.492253
 H56     -C24     -H54     : 109.797905  H56     -C24     -H55     :
107.948708
 C26     -P25     -Co20    : 116.312564  C27     -P25     -Co20    :
116.332067
 C27     -P25     -C26     : 101.600421  C28     -P25     -Co20    :
116.510555
 C28     -P25     -C26     : 102.106813  C28     -P25     -C27     :
101.562139
 H45     -C26     -P25     : 110.805075  H46     -C26     -P25     :
109.545912
 H46     -C26     -H45     : 109.819675  H47     -C26     -P25     :
109.109673
 H47     -C26     -H45     : 109.591027  H47     -C26     -H46     :
107.915120
 H51     -C27     -P25     : 110.607670  H52     -C27     -P25     :
109.212387
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Co17    -Se31   -Co22   -Se33   : 120.197954
Co17    -Se32   -Co10   -Se31   : -41.551756
Co17    -Se32   -Co10   -Se33   :  37.578897
Co17    -Se32   -Co14   -Se30   :  40.920814
P18     -Co17   -Se29   -Co20   : 138.045887
P18     -Co17   -Se29   -Co22   :-143.227657
P18     -Co17   -Se30   -Co20   :-139.756022
P18     -Co17   -Se31   -Co22   : 139.516542
C19     -P18    -Co17   -Se29   : -40.862320
C19     -P18    -Co17   -Se30   :  49.198663
C19     -P18    -Co17   -Se31   :-130.604480
C19     -P18    -Co17   -Se32   : 139.638807
C19     -P18    -C43    -H69    :  50.831488
C19     -P18    -C43    -H70    : 172.182005
C19     -P18    -C43    -H71    : -69.844126
C19     -P18    -C44    -H63    : -50.904404
C19     -P18    -C44    -H64    :  69.906300
C19     -P18    -C44    -H65    :-172.134596
Co20    -Se13   -Co12   -Se21   :  41.447732
Co20    -Se13   -Co12   -Se33   : -38.293637
Co20    -Se13   -Co12   -P34    : 143.099909
Co20    -Se13   -Co14   -Se30   : -41.187809
Co20    -Se13   -Co14   -Se32   :  43.161148
Co20    -Se21   -Co12   -Se33   : 120.071343
Co20    -Se21   -Co12   -P34    :-142.921861
Co20    -Se21   -Co22   -P23    : 143.285340
Co20    -Se21   -Co22   -Se29   :  41.783907
Co20    -Se21   -Co22   -Se31   : -36.240810
Co20    -Se21   -Co22   -Se33   :-119.841444
Co20    -P25    -C26    -H45    : 178.017897
Co20    -P25    -C26    -H46    : -60.664107
Co20    -P25    -C26    -H47    :  57.270191
Co20    -P25    -C27    -H51    : 179.465113
Co20    -P25    -C27    -H52    : -59.684505
Co20    -P25    -C27    -H53    :  58.591012
Co20    -P25    -C28    -H48    :-178.192343
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Co20    -P25    -C28    -H49    : -57.424992
Co20    -P25    -C28    -H50    :  60.513339
Co20    -Se29   -Co17   -Se30   :  41.235297
Co20    -Se29   -Co17   -Se31   :-120.162432
Co20    -Se29   -Co17   -Se32   : -43.400758
Co20    -Se29   -Co22   -Se21   : -41.562548
Co20    -Se29   -Co22   -P23    :-139.610465
Co20    -Se29   -Co22   -Se31   : 118.929130
Co20    -Se29   -Co22   -Se33   :  38.487930
Co20    -Se30   -Co14   -Se32   :-118.872398
Co20    -Se30   -Co17   -Se29   : -41.343110
Co20    -Se30   -Co17   -Se31   :  39.647323
Co20    -Se30   -Co17   -Se32   : 118.890706
Se21    -Co12   -Se33   -Co22   : -41.199135
Se21    -Co12   -P34    -C35    : 102.309751
Se21    -Co12   -P34    -C36    : -18.343107
Se21    -Co12   -P34    -C37    :-137.941497
Se21    -Co20   -P25    -C26    : 105.915476
Se21    -Co20   -P25    -C27    :-134.411952
Se21    -Co20   -P25    -C28    : -14.624182
Se21    -Co20   -Se29   -Co22   :  41.684787
Se21    -Co22   -P23    -C24    : 161.680782
Se21    -Co22   -P23    -C41    :  42.275929
Se21    -Co22   -P23    -C42    : -77.641691
Co22    -Se21   -Co12   -Se33   :  41.243971
Co22    -Se21   -Co12   -P34    : 138.250767
Co22    -Se21   -Co20   -P25    :-143.099009
Co22    -Se21   -Co20   -Se29   : -41.535393
Co22    -Se21   -Co20   -Se30   :  38.113263
Co22    -P23    -C24    -H54    :-177.293019
Co22    -P23    -C24    -H55    : -56.501549
Co22    -P23    -C24    -H56    :  61.435367
Co22    -P23    -C41    -H60    : 179.525865
Co22    -P23    -C41    -H61    : -59.527549
Co22    -P23    -C41    -H62    :  58.679118
Co22    -P23    -C42    -H57    : 177.936855
Co22    -P23    -C42    -H58    : -60.859200
Co22    -P23    -C42    -H59    :  57.097796
Co22    -Se29   -Co17   -Se30   : 119.961753
Co22    -Se29   -Co17   -Se31   : -41.435976
Co22    -Se29   -Co17   -Se32   :  35.325698
Co22    -Se29   -Co20   -P25    : 142.971082
Co22    -Se29   -Co20   -Se30   :-120.105759
Co22    -Se31   -Co10   -Se32   : 120.139937
Co22    -Se31   -Co10   -Se33   : -41.141897
Co22    -Se31   -Co17   -Se29   :  41.284014
Co22    -Se31   -Co17   -Se30   : -39.877963
Co22    -Se31   -Co17   -Se32   :-119.390455
Co22    -Se33   -Co10   -Se31   :  41.135093
Co22    -Se33   -Co10   -Se32   : -37.745166
Co22    -Se33   -Co12   -P34    :-142.966859
C24     -P23    -Co22   -Se29   :-108.846010
C24     -P23    -Co22   -Se31   : -18.484264
C24     -P23    -Co22   -Se33   :  71.766888
C24     -P23    -C41    -H60    :  52.426286
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C24	-P23	-C41	-H61	: 173.372872
C24	-P23	-C41	-H62	: -68.420462
C24	-P23	-C42	-H57	: -54.102404
C24	-P23	-C42	-H58	: 67.101541
C24	-P23	-C42	-H59	:-174.941463
C26	-P25	-Co20	-Se29	: 15.915123
C26	-P25	-Co20	-Se30	: -74.472410
C26	-P25	-C27	-H51	: -53.198178
C26	-P25	-C27	-H52	: 67.652204
C26	-P25	-C27	-H53	:-174.072278
C26	-P25	-C28	-H48	: 53.956002
C26	-P25	-C28	-H49	: 174.723352
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C27	-P25	-Co20	-Se30	: 45.200162
C27	-P25	-C26	-H45	: 50.668541
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C27	-P25	-C26	-H47	: -70.079164
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C27	-P25	-C28	-H50	:-172.040988
C28	-P25	-Co20	-Se29	:-104.624536
C28	-P25	-Co20	-Se30	: 164.987932
C28	-P25	-C26	-H45	: -54.004200
C28	-P25	-C26	-H46	: 67.313796
C28	-P25	-C26	-H47	:-174.751906
C28	-P25	-C27	-H51	: 51.903879
C28	-P25	-C27	-H52	: 172.754260
C28	-P25	-C27	-H53	: -68.970222
Se29	-Co17	-P18	-C43	:-160.378746
Se29	-Co17	-P18	-C44	: 78.953180
Se29	-Co22	-P23	-C41	: 131.749137
Se29	-Co22	-P23	-C42	: 11.831518
Se30	-Co14	-P15	-C38	: 162.159870
Se30	-Co14	-P15	-C39	: -77.161775
Se30	-Co17	-P18	-C43	: -70.317763
Se30	-Co17	-P18	-C44	: 169.014162
Se31	-Co10	-P7	-C40	: 149.026912
Se31	-Co17	-P18	-C43	: 109.879095
Se31	-Co17	-P18	-C44	: -10.788980
Se31	-Co22	-P23	-C41	:-137.889117
Se31	-Co22	-P23	-C42	: 102.193264
Se32	-Co10	-P7	-C40	:-121.308692
Se32	-Co14	-P15	-C38	: 72.165212
Se32	-Co14	-P15	-C39	:-167.156434
Se32	-Co17	-P18	-C43	: 20.122382
Se32	-Co17	-P18	-C44	:-100.545693
Se33	-Co10	-P7	-C40	: 59.106682
Se33	-Co12	-P34	-C35	:-167.506021
Se33	-Co12	-P34	-C36	: 71.841121
Se33	-Co12	-P34	-C37	: -47.757269
Se33	-Co22	-P23	-C41	: -47.637965
Se33	-Co22	-P23	-C42	:-167.555584
C35	-P34	-C36	-H72	: 54.212641
C35	-P34	-C36	-H73	: 175.002476

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C35     -P34     -C36     -H74     : -67.075452
C35     -P34     -C37     -H78     : -52.782454
C35     -P34     -C37     -H79     :  68.123349
C35     -P34     -C37     -H80     :-173.622135
C36     -P34     -C35     -H75     : -53.802703
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C36     -P34     -C35     -H77     :-174.640848
C36     -P34     -C37     -H78     :  52.339034
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C37     -P34     -C36     -H73     :  70.304059
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C38     -P15     -C16     -H81     :  52.289172
C38     -P15     -C16     -H82     : 173.188747
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C38     -P15     -C39     -H86     :-174.604772
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C39     -P15     -C38     -H87     :  54.664827
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C40     -P7      -C8      -H95     :  52.992548
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C41     -P23     -C24     -H55     :  70.387264
C41     -P23     -C24     -H56     :-171.675819
C41     -P23     -C42     -H57     :  50.666645
C41     -P23     -C42     -H58     : 171.870590
C41     -P23     -C42     -H59     : -70.172414
C42     -P23     -C24     -H54     :  54.379193
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C42     -P23     -C41     -H60     : -52.622603
C42     -P23     -C41     -H61     :  68.323983
C42     -P23     -C41     -H62     :-173.469351
C43     -P18     -C19     -H66     : -52.170927
C43     -P18     -C19     -H67     :  68.638643
C43     -P18     -C19     -H68     :-173.091811
C43     -P18     -C44     -H63     :  53.717837
C43     -P18     -C44     -H64     : 174.528540
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C44     -P18     -C19     -H66     :  52.814436
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C44     -P18     -C19     -H68     : -68.106449
C44     -P18     -C43     -H69     : -53.753985
C44     -P18     -C43     -H70     :  67.596532
C44     -P18     -C43     -H71     :-174.429599
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H96     -C3      -C4      -H97     :  -0.422818
H98     -C6      -C1      -H99     :   1.482237
C100    -C102    -C104    -C105    :-178.046017
C100    -C102    -C104    -H109    :   1.333017
C100    -C102    -C108    -C107    : 177.887536
C100    -C102    -C108    -H113    :  -1.067633
H101    -C9      -C100    -C102    :   2.458276
H101    -C9      -C100    -H103    : 179.962262
C102    -C104    -C105    -C106    :  -0.148513
C102    -C104    -C105    -H110    : 179.705707
C102    -C108    -C107    -C106    :   0.288966
C102    -C108    -C107    -H112    :-179.535700
H103    -C100    -C102    -C104    :   2.516814
H103    -C100    -C102    -C108    :-175.677013
C104    -C102    -C108    -C107    :  -0.342003
C104    -C102    -C108    -H113    :-179.297173
C104    -C105    -C106    -C107    :   0.079259
C104    -C105    -C106    -S111    : 179.071890
C105    -C104    -C102    -C108    :   0.272606
C105    -C106    -C107    -C108    :  -0.148244
C105    -C106    -C107    -H112    : 179.673179
C105    -C106    -S111    -C114    :-178.310877
C106    -C105    -C104    -H109    :-179.527091
C106    -C107    -C108    -H113    : 179.260666
C106    -S111    -C114    -H115    :-179.876629
C106    -S111    -C114    -H116    : -61.578556
C106    -S111    -C114    -H117    :  62.051325
C107    -C106    -C105    -H110    :-179.774969
C107    -C106    -S111    -C114    :   0.614410
C108    -C102    -C104    -H109    : 179.651640
C108    -C107    -C106    -S111    :-179.055506
H109    -C104    -C105    -H110    :   0.327128
H110    -C105    -C106    -S111    :  -0.782338
S111    -C106    -C107    -H112    :   0.765917
H112    -C107    -C108    -H113    :  -0.564000
```

co6se8_pme3_4_bis_4-thiomethylphenyl-dimethylphosphine

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion............   12399.28085583093
   (E)  Total one-electron terms.....  -31950.07645839576
   (I)  Total two-electron terms.....   14580.71646143610
   (J)    Coulomb....................   15064.15431269327
   (K)    Exchange+Correlation.......    -483.43785125717
   (L)  Electronic energy............  -17369.35999695967  (E+I)
   (N)  Total energy.................   -4970.07914112874  (A+L)

 SCFE: SCF energy: DFT(b3lyp)     -4970.07914112874 hartrees


 HOMO energy:    -0.15753
 LUMO energy:    -0.05742

  Orbital energies (hartrees):
   -88.86459   -88.86431   -77.09495   -77.09488   -77.09038   -77.09029
   -77.09015   -77.09013   -10.21811   -10.21784   -10.21388   -10.21371
   -10.18976   -10.18939   -10.18830   -10.18790   -10.18772   -10.18758
   -10.18704   -10.18695   -10.18664   -10.18638   -10.17490   -10.17418
   -10.17355   -10.17322   -10.17312   -10.17311   -10.17258   -10.17236
   -10.17175   -10.17173   -10.17164   -10.17146   -10.17136   -10.17121
   -10.17090   -10.17081    -7.94054    -7.94026    -6.57169    -6.57165
    -6.56761    -6.56754    -6.56738    -6.56733    -5.90505    -5.90477
    -5.90090    -5.90062    -5.89460    -5.89432    -4.73369    -4.73367
    -4.73349    -4.73344    -4.73049    -4.73046    -4.72944    -4.72941
    -4.72937    -4.72934    -4.72923    -4.72917    -4.72916    -4.72914
    -4.72651    -4.72644    -4.72628    -4.72625    -3.70092    -3.70092
    -3.70064    -3.70061    -3.70041    -3.70002    -2.39529    -2.39515
    -2.39508    -2.39499    -2.39477    -2.39447    -2.39179    -2.39145
    -2.39132    -2.39131    -2.39125    -2.39119    -2.39100    -2.39098
    -2.39071    -2.39065    -2.39064    -2.38983    -0.86160    -0.86131
    -0.80202    -0.80173    -0.76335    -0.76312    -0.76297    -0.76274
    -0.76036    -0.76020    -0.74654    -0.74624    -0.72491    -0.72484
    -0.68864    -0.68844    -0.68739    -0.68717    -0.68716    -0.68687
    -0.68623    -0.68612    -0.68581    -0.68578    -0.65428    -0.65397
    -0.64313    -0.61488    -0.61405    -0.61390    -0.60618    -0.60590
    -0.59290    -0.59215    -0.59015    -0.58673    -0.58629    -0.57914
    -0.55128    -0.55095    -0.53715    -0.53628    -0.53613    -0.53579
    -0.49026    -0.49010    -0.46060    -0.46033    -0.44974    -0.44956
    -0.44029    -0.43985    -0.43890    -0.43739    -0.43696    -0.43679
    -0.43565    -0.43542    -0.42858    -0.42795    -0.42239    -0.42228
    -0.42154    -0.42142    -0.42133    -0.42123    -0.42086    -0.42056
    -0.42044    -0.42026    -0.41156    -0.41143    -0.40166    -0.40129
    -0.39936    -0.39912    -0.39896    -0.39881    -0.39813    -0.39755
    -0.39730    -0.39660    -0.39052    -0.39035    -0.38077    -0.38076
    -0.38059    -0.38052    -0.38029    -0.38002    -0.37121    -0.37099
    -0.35271    -0.35259    -0.33742    -0.33683    -0.33338    -0.33263
    -0.33174    -0.33136    -0.33098    -0.33075    -0.33056    -0.33043
    -0.33039    -0.32970    -0.32764    -0.32628    -0.31869    -0.31856
    -0.31559    -0.31071    -0.30803    -0.30762    -0.29369    -0.29347
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-0.28426	-0.28306	-0.28145	-0.28014	-0.27964	-0.27837
-0.27809	-0.27734	-0.27575	-0.27481	-0.27062	-0.26952
-0.25360	-0.25308	-0.25212	-0.25069	-0.24981	-0.23758
-0.23660	-0.23596	-0.23557	-0.23053	-0.23010	-0.22859
-0.22788	-0.22717	-0.22676	-0.22627	-0.22560	-0.22024
-0.21491	-0.21450	-0.20711	-0.20674	-0.19740	-0.19683
-0.19523	-0.19154	-0.18985	-0.18954	-0.18089	-0.17986
-0.17886	-0.16939	-0.16033	-0.15877	-0.15753	-0.05742
-0.05233	-0.05206	-0.04720	-0.04376	-0.03537	-0.03457
-0.03405	-0.03134	-0.03067			

final geometry:

		angstroms	
atom	x	y	z
Co1	-0.0090103900	-0.0306981324	-0.0479516752
Co2	-0.2963881934	-0.0969055880	2.8937529589
Co3	2.3919900419	-0.0464205178	1.7043109042
Co4	1.4386645607	-2.5164625394	3.0259356665
Co5	1.7497502607	-2.4337296050	0.0896175471
Co6	-0.9558460435	-2.4969889726	1.2714990702
Se7	1.8187558822	-0.3557994495	4.0326598261
Se8	3.4836323340	-2.2006877881	1.7586874878
Se9	0.7580382065	-4.2003594649	1.4205911943
Se10	-0.3652498241	-2.2005873676	-1.0626340565
Se11	-2.0470692480	-0.3378700183	1.2346689443
Se12	0.6845532966	1.6583021214	1.5426524123
Se13	2.3036482333	-0.2209430888	-0.7035753268
Se14	-0.8767594412	-2.3091594266	3.6865208874
P15	-2.7162892093	-3.7491684541	0.9472851446
P16	2.9192682487	-3.6402694242	-1.3053274129
P17	2.1424601476	-3.9016207492	4.5700696043
P18	4.1317221518	1.2281795614	2.0378635381
P19	-1.3194265513	1.2093099035	4.3158588712
P20	-0.8507477704	1.2882109946	-1.5810812493
C21	0.9366631627	-5.2121377737	5.0654134314
C22	3.5957527837	-4.9358530438	4.0977775685
C23	2.6391488216	-3.1901638592	6.1925356197
C24	1.6620510148	-2.8258718654	7.1329452939
C25	2.0119184759	-2.2551645036	8.3485317382
C26	3.3583396258	-2.0170107466	8.6669927746
C27	4.3383553066	-2.3689376134	7.7342127938
C28	3.9772590663	-2.9459732857	6.5160682794
S29	3.6874917829	-1.2827483606	10.2576747403
C30	5.4816080231	-0.9721135528	10.2201189783
C31	5.4713176966	0.5139131572	3.0866839159
C32	3.8142592632	2.8311983660	2.8946626786
C33	5.0618609695	1.7709091066	0.5406317747
C34	-0.2473994509	2.3349347768	5.3101319839
C35	-2.3293788632	0.3884053016	5.6235133780
C36	-2.5326192884	2.3991193351	3.5959054269
C37	-4.0143792104	-3.0548107963	-0.1651434321
C38	-2.4118966590	-5.3966020657	0.1751517537
C39	-3.7007497651	-4.1971946186	2.4418839711
C40	2.0722012459	-4.1880227373	-2.8500623255

C41	4.4565874696	-2.8612633187	-1.9637982207
C42	3.5670545105	-5.2374286254	-0.6458239430
H43	1.3658501307	-5.8662496456	5.8311601564
H44	0.6847315123	-5.7919929859	4.1742206155
H45	0.0189582118	-4.7548915987	5.4384051356
H46	3.3114977584	-5.5142055534	3.2152263176
H47	3.8786083911	-5.6121975912	4.9107974030
H48	1.2333224501	-1.9828638025	9.0567560021
H49	4.4404057008	-4.3036856180	3.8211657329
H50	0.6092560600	-2.9724020874	6.9086739119
H51	4.7669160532	-3.1996070992	5.8153398646
H52	5.3900192302	-2.2030545898	7.9410192236
H53	5.7543312014	-0.3162117002	9.3898384615
H54	5.7126499095	-0.4680483830	11.1612319512
H55	6.0522069472	-1.9023823997	10.1699140134
H56	5.4197388266	0.8922833413	-0.0009426809
H57	4.3908791467	2.3207189914	-0.1232283341
H58	5.9116131276	2.4049518573	0.8178746073
H59	4.7517824812	3.3729930488	3.0623986202
H60	3.3299252853	2.6309626780	3.8533457772
H61	3.1380630673	3.4397919179	2.2910438185
H62	6.2729282863	1.2446544053	3.2423008187
H63	5.0479181802	0.2202816287	4.0502391795
H64	5.8737355190	-0.3795308338	2.6050353707
H65	0.4383069622	1.7419941557	5.9187735197
H66	0.3455532093	2.9520925934	4.6309065351
H67	-0.8551497757	2.9786276725	5.9558054325
H68	-2.9639151298	3.0331904929	4.3785218144
H69	-2.0243388418	3.0231607837	2.8571768365
H70	-3.3262993803	1.8468019707	3.0887254912
H71	-2.8025321947	1.1329022492	6.2737116032
H72	-1.6893396360	-0.2664873904	6.2188932766
H73	-3.0970324412	-0.2299370633	5.1526265826
H74	4.1784738103	-5.0352752615	0.2367183600
H75	2.7310725872	-5.8717004583	-0.3441494833
H76	4.1704477156	-5.7527335269	-1.4013957206
H77	5.0951294816	-2.5743677497	-1.1248768464
H78	4.9959629142	-3.5566902951	-2.6165222178
H79	4.1976230559	-1.9570355641	-2.5183439016
H80	-3.0681186857	-4.7437132031	3.1448180129
H81	-4.5662736183	-4.8112893013	2.1688999635
H82	-4.0394360164	-3.2840821392	2.9369132144
H83	-4.4012233272	-2.1279780956	0.2631736832
H84	-4.8325611052	-3.7710556742	-0.2996438026
H85	-3.5656280240	-2.8234182761	-1.1339174808
H86	-1.7618901556	-5.9884065002	0.8226744695
H87	-3.3553742085	-5.9283464470	0.0089973477
H88	-1.8991168240	-5.2513980787	-0.7786567519
H89	1.7393537778	-3.3126561377	-3.4121307777
H90	1.1885094503	-4.7746775556	-2.5888645252
H91	2.7455888456	-4.7908446288	-3.4697331856
C92	0.2942047881	1.9586976983	-2.8595630572
C93	-1.6954368328	2.7983757603	-0.9394800054
C94	-2.2027873729	0.5495626416	-2.6016632561
C95	0.8210145730	3.2510340279	-2.7791263074

C96	1.7228746034	3.7300963202	-3.7308030373
C97	2.1236130222	2.9177782753	-4.7954143706
C98	1.5997636600	1.6180899929	-4.8834935234
C99	0.7077337461	1.1490412832	-3.9296973764
S100	3.2646463330	3.4102323031	-6.0736234670
C101	3.8472329363	5.0432979096	-5.5165074730
H102	-2.5012923157	2.4689307669	-0.2794963310
H103	-2.1055268278	3.3953098686	-1.7601170086
H104	-1.0023368097	3.3975456060	-0.3475452488
H105	-2.9941696632	0.2210418333	-1.9232377980
H106	-1.8354054295	-0.3269884065	-3.1370487617
H107	-2.5988840205	1.2823779952	-3.3120766482
H108	0.5394912426	3.9093504818	-1.9632190513
H109	2.1013512189	4.7412576684	-3.6280014107
H110	1.9042283572	0.9672591926	-5.6992471447
H111	0.3435075163	0.1289513086	-4.0124403053
H112	4.3105062036	4.9841075959	-4.5286330552
H113	4.6018327600	5.3505567759	-6.2441269330
H114	3.0411976958	5.7807857179	-5.5117710632

bond lengths (angstroms):

Co1	-Se10	:	2.421757	Co1	-Se11	:	2.427582
Co1	-Se12	:	2.421523	Co1	-Se13	:	2.411312
Co1	-P20	:	2.190555	Co2	-Se7	:	2.416189
Co2	-Se11	:	2.423945	Co2	-Se12	:	2.422493
Co2	-Se14	:	2.420615	Co2	-P19	:	2.185221
Co3	-Se7	:	2.417751	Co3	-Se8	:	2.415679
Co3	-Se12	:	2.418171	Co3	-Se13	:	2.415818
Co3	-P18	:	2.182322	Co4	-Se7	:	2.413799
Co4	-Se8	:	2.426422	Co4	-Se9	:	2.424024
Co4	-Se14	:	2.416720	Co4	-P17	:	2.190512
Co5	-Se8	:	2.417943	Co5	-Se9	:	2.424039
Co5	-Se10	:	2.419765	Co5	-Se13	:	2.415033
Co5	-P16	:	2.183892	Co6	-Se9	:	2.420971
Co6	-Se10	:	2.425868	Co6	-Se11	:	2.419487
Co6	-Se14	:	2.423606	Co6	-P15	:	2.184543
P15	-C37	:	1.845174	P15	-C38	:	1.844690
P15	-C39	:	1.844916	P16	-C40	:	1.844929
P16	-C41	:	1.844935	P16	-C42	:	1.845397
P17	-C21	:	1.848450	P17	-C22	:	1.845198
P17	-C23	:	1.839909	P18	-C31	:	1.845187
P18	-C32	:	1.845144	P18	-C33	:	1.844293
P19	-C34	:	1.845224	P19	-C35	:	1.844952
P19	-C36	:	1.845485	P20	-C92	:	1.842548
P20	-C93	:	1.845467	P20	-C94	:	1.848026
C21	-H43	:	1.094729	C21	-H44	:	1.092669
C21	-H45	:	1.091045	C22	-H46	:	1.092790
C22	-H47	:	1.094738	C22	-H49	:	1.090682
C23	-C24	:	1.404208	C23	-C28	:	1.398156
C24	-C25	:	1.387719	C24	-H50	:	1.086345
C25	-C26	:	1.403918	C25	-H48	:	1.087171
C26	-C27	:	1.397985	C26	-S29	:	1.782625
C27	-C28	:	1.395434	C27	-H52	:	1.084566
C28	-H51	:	1.085776	S29	-C30	:	1.821197

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 C30     -H53     :   1.092681      C30     -H54     :   1.092317
 C30     -H55     :   1.092476      C31     -H62     :   1.095801
 C31     -H63     :   1.092669      C31     -H64     :   1.091864
 C32     -H59     :   1.095731      C32     -H60     :   1.092587
 C32     -H61     :   1.091780      C33     -H56     :   1.092411
 C33     -H57     :   1.092345      C33     -H58     :   1.095880
 C34     -H65     :   1.091887      C34     -H66     :   1.092622
 C34     -H67     :   1.095717      C35     -H71     :   1.095859
 C35     -H72     :   1.092251      C35     -H73     :   1.092416
 C36     -H68     :   1.095696      C36     -H69     :   1.092473
 C36     -H70     :   1.091886      C37     -H83     :   1.091844
 C37     -H84     :   1.095682      C37     -H85     :   1.092448
 C38     -H86     :   1.091800      C38     -H87     :   1.095678
 C38     -H88     :   1.092601      C39     -H80     :   1.092255
 C39     -H81     :   1.095794      C39     -H82     :   1.092491
 C40     -H89     :   1.092234      C40     -H90     :   1.092382
 C40     -H91     :   1.095827      C41     -H77     :   1.092627
 C41     -H78     :   1.095716      C41     -H79     :   1.091884
 C42     -H74     :   1.092511      C42     -H75     :   1.091867
 C42     -H76     :   1.095678      C92     -C95     :   1.397903
 C92     -C99     :   1.404186      C93     -H102    :   1.092481
 C93     -H103    :   1.094509      C93     -H104    :   1.090770
 C94     -H105    :   1.092919      C94     -H106    :   1.090848
 C94     -H107    :   1.094805      C95     -C96     :   1.395901
 C95     -H108    :   1.085514      C96     -C97     :   1.397802
 C96     -H109    :   1.084555      C97     -C98     :   1.404053
 C97     -S100    :   1.782775      C98     -C99     :   1.387606
 C98     -H110    :   1.087076      C99     -H111    :   1.086320
 S100    -C101    :   1.821178      C101    -H112    :   1.092713
 C101    -H113    :   1.092364      C101    -H114    :   1.092522

  bond angles:

 Se11    -Co1     -Se10    :  89.111990  Se12    -Co1     -Se10    :
160.441721
 Se12    -Co1     -Se11    :  88.949196  Se13    -Co1     -Se10    :
87.505109
 Se13    -Co1     -Se11    : 159.862349  Se13    -Co1     -Se12    :
87.646152
 P20     -Co1     -Se10    : 100.935611  P20     -Co1     -Se11    :
97.086572
 P20     -Co1     -Se12    :  98.616996  P20     -Co1     -Se13    :
103.046702
 Se11    -Co2     -Se7     : 160.775133  Se12    -Co2     -Se7     :
89.200794
 Se12    -Co2     -Se11    :  89.011216  Se14    -Co2     -Se7     :
87.569189
 Se14    -Co2     -Se11    :  87.715832  Se14    -Co2     -Se12    :
160.377612
 P19     -Co2     -Se7     :  99.620636  P19     -Co2     -Se11    :
99.597596
 P19     -Co2     -Se12    :  96.859695  P19     -Co2     -Se14    :
102.762677
 Se8     -Co3     -Se7     :  88.358298  Se12    -Co3     -Se7     :
89.265391
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Se12 -Co3 -Se8 : 161.669856 Se13 -Co3 -Se7 : 160.381021
Se13 -Co3 -Se8 : 88.540921 Se13 -Co3 -Se12 : 87.620134
P18 -Co3 -Se7 : 96.693331 P18 -Co3 -Se8 : 99.042222
P18 -Co3 -Se12 : 99.286183 P18 -Co3 -Se13 : 102.925630
Se8 -Co4 -Se7 : 88.201777 Se9 -Co4 -Se7 : 160.431948
Se9 -Co4 -Se8 : 88.920801 Se14 -Co4 -Se7 : 87.712201
Se14 -Co4 -Se8 : 159.894282 Se14 -Co4 -Se9 : 88.372364
P17 -Co4 -Se7 : 102.793430 P17 -Co4 -Se8 : 100.350479
P17 -Co4 -Se9 : 96.764330 P17 -Co4 -Se14 : 99.752079
Se9 -Co5 -Se8 : 89.117459 Se10 -Co5 -Se8 : 161.118407
Se10 -Co5 -Se9 : 88.515294 Se13 -Co5 -Se8 : 88.506741
Se13 -Co5 -Se9 : 160.378753 Se13 -Co5 -Se10 : 87.466102
P16 -Co5 -Se8 : 96.323730 P16 -Co5 -Se9 : 99.623097
P16 -Co5 -Se10 : 102.541341 P16 -Co5 -Se13 : 99.996814
Se10 -Co6 -Se9 : 88.445397 Se11 -Co6 -Se9 : 161.459585
Se11 -Co6 -Se10 : 89.204770 Se14 -Co6 -Se9 : 88.284402
Se14 -Co6 -Se10 : 160.281756 Se14 -Co6 -Se11 : 87.749172
P15 -Co6 -Se9 : 100.156604 P15 -Co6 -Se10 : 97.090035
P15 -Co6 -Se11 : 98.383663 P15 -Co6 -Se14 : 102.627218
Co3 -Se7 -Co2 : 74.924427 Co4 -Se7 -Co2 : 76.200438
Co4 -Se7 -Co3 : 75.535989 Co4 -Se8 -Co3 : 75.342341
Co5 -Se8 -Co3 : 75.307009 Co5 -Se8 -Co4 : 75.144357
Co5 -Se9 -Co4 : 75.077368 Co6 -Se9 -Co4 : 75.569687
Co6 -Se9 -Co5 : 75.110179 Co5 -Se10 -Co1 : 76.009668
Co6 -Se10 -Co1 : 75.057289 Co6 -Se10 -Co5 : 75.098750
Co2 -Se11 -Co1 : 75.090121 Co6 -Se11 -Co1 : 75.067222
Co6 -Se11 -Co2 : 75.673370 Co2 -Se12 -Co1 : 75.226776

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 Co3     -Se12    -Co1     :  75.784960  Co3     -Se12    -Co2     :
74.802448
 Co3     -Se13    -Co1     :  76.017241  Co5     -Se13    -Co1     :
76.291504
 Co5     -Se13    -Co3     :  75.357765  Co4     -Se14    -Co2     :
76.064005
 Co6     -Se14    -Co2     :  75.658906  Co6     -Se14    -Co4     :
75.655280
 C37     -P15     -Co6     : 116.148823  C38     -P15     -Co6     :
116.171014
 C38     -P15     -C37     : 101.525601  C39     -P15     -Co6     :
116.678304
 C39     -P15     -C37     : 101.794200  C39     -P15     -C38     :
102.137953
 C40     -P16     -Co5     : 116.933979  C41     -P16     -Co5     :
116.162972
 C41     -P16     -C40     : 102.070023  C42     -P16     -Co5     :
115.967783
 C42     -P16     -C40     : 101.738023  C42     -P16     -C41     :
101.565797
 C21     -P17     -Co4     : 115.317568  C22     -P17     -Co4     :
115.280631
 C22     -P17     -C21     : 100.660345  C23     -P17     -Co4     :
117.634494
 C23     -P17     -C21     : 102.353310  C23     -P17     -C22     :
103.286774
 C31     -P18     -Co3     : 116.075061  C32     -P18     -Co3     :
116.182302
 C32     -P18     -C31     : 101.377245  C33     -P18     -Co3     :
116.733660
 C33     -P18     -C31     : 102.076324  C33     -P18     -C32     :
102.010072
 C34     -P19     -Co2     : 116.315591  C35     -P19     -Co2     :
116.844496
 C35     -P19     -C34     : 101.978612  C36     -P19     -Co2     :
116.056601
 C36     -P19     -C34     : 101.469307  C36     -P19     -C35     :
101.742053
 C92     -P20     -Co1     : 117.771260  C93     -P20     -Co1     :
115.166557
 C93     -P20     -C92     : 103.172020  C94     -P20     -Co1     :
115.276610
 C94     -P20     -C92     : 102.525612  C94     -P20     -C93     :
100.614930
 H43     -C21     -P17     : 110.813417  H44     -C21     -P17     :
107.943526
 H44     -C21     -H43     : 110.109476  H45     -C21     -P17     :
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 H45     -C21     -H43     : 109.940363  H45     -C21     -H44     :
107.896442
 H46     -C22     -P17     : 107.366569  H47     -C22     -P17     :
111.081462
 H47     -C22     -H46     : 109.877950  H49     -C22     -P17     :
110.486636
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 H49     -C22     -H46     : 107.660414  H49     -C22     -H47     :
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 C24     -C23     -P17     : 120.200964  C28     -C23     -P17     :
122.001804
 C28     -C23     -C24     : 117.753718  C25     -C24     -C23     :
121.191319
 H50     -C24     -C23     : 120.072443  H50     -C24     -C25     :
118.727243
 C26     -C25     -C24     : 120.680853  H48     -C25     -C24     :
119.543329
 H48     -C25     -C26     : 119.773884  C27     -C26     -C25     :
118.571403
 S29     -C26     -C25     : 116.703153  S29     -C26     -C27     :
124.725090
 C28     -C27     -C26     : 120.341671  H52     -C27     -C26     :
120.932105
 H52     -C27     -C28     : 118.726021  C27     -C28     -C23     :
121.458320
 H51     -C28     -C23     : 120.391370  H51     -C28     -C27     :
118.149679
 C30     -S29     -C26     : 103.518197  H53     -C30     -S29     :
111.342030
 H54     -C30     -S29     : 105.623429  H54     -C30     -H53     :
108.958226
 H55     -C30     -S29     : 111.730352  H55     -C30     -H53     :
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110.711908
 H63     -C31     -P18     : 108.902040  H63     -C31     -H62     :
109.720568
 H64     -C31     -P18     : 109.486502  H64     -C31     -H62     :
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 H60     -C32     -P18     : 108.934970  H60     -C32     -H59     :
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 H61     -C32     -P18     : 109.518800  H61     -C32     -H59     :
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 H57     -C33     -P18     : 109.371992  H57     -C33     -H56     :
107.744223
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 H58     -C33     -H57     : 109.806090  H65     -C34     -P19     :
109.508361
 H66     -C34     -P19     : 108.958680  H66     -C34     -H65     :
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 H67     -C34     -P19     : 110.710209  H67     -C34     -H65     :
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110.769019
 H72     -C35     -P19     : 109.411813  H72     -C35     -H71     :
109.689837
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 H73     -C35     -P19     : 109.330098  H73     -C35     -H71     :
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 H70     -C36     -P19     : 109.446921  H70     -C36     -H68     :
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 H84     -C37     -P15     : 110.692038  H84     -C37     -H83     :
109.784854
 H85     -C37     -P15     : 108.987233  H85     -C37     -H83     :
108.277350
 H85     -C37     -H84     : 109.654171  H86     -C38     -P15     :
109.516416
 H87     -C38     -P15     : 110.781269  H87     -C38     -H86     :
109.848258
 H88     -C38     -P15     : 108.914441  H88     -C38     -H86     :
108.081217
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  torsional angles:

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Se13	-Co1	-P20	-C93	:-124.710666
Se13	-Co1	-P20	-C94	: 118.741813
Se13	-Co3	-P18	-C31	:-122.222715
Se13	-Co3	-P18	-C32	: 118.742727
Se13	-Co3	-P18	-C33	: -1.739932
Se13	-Co5	-P16	-C40	: -91.547274
Se13	-Co5	-P16	-C41	: 29.177790
Se13	-Co5	-P16	-C42	: 148.368996
Se14	-Co2	-P19	-C34	: 118.892898
Se14	-Co2	-P19	-C35	: -1.758629
Se14	-Co2	-P19	-C36	:-121.848454
Se14	-Co4	-P17	-C21	: 37.174977
Se14	-Co4	-P17	-C22	: 153.902116
Se14	-Co4	-P17	-C23	: -83.810813
Se14	-Co6	-P15	-C37	: 124.663931
Se14	-Co6	-P15	-C38	:-116.042616
Se14	-Co6	-P15	-C39	: 4.563262
P17	-C23	-C24	-C25	:-178.291135
P17	-C23	-C24	-H50	: 0.603907
P17	-C23	-C28	-C27	: 178.054539
P17	-C23	-C28	-H51	: -1.651171
P20	-C92	-C95	-C96	: 177.797461
P20	-C92	-C95	-H108	: -1.829945
P20	-C92	-C99	-C98	:-178.099963
P20	-C92	-C99	-H111	: 0.747396
C21	-P17	-C22	-H46	: 65.852492
C21	-P17	-C22	-H47	: -54.304611
C21	-P17	-C22	-H49	:-177.007172
C21	-P17	-C23	-C24	: -48.712737
C21	-P17	-C23	-C28	: 133.740886
C22	-P17	-C21	-H43	: 54.734300
C22	-P17	-C21	-H44	: -65.910972
C22	-P17	-C21	-H45	: 176.559331
C22	-P17	-C23	-C24	:-152.971288
C22	-P17	-C23	-C28	: 29.482335
C23	-P17	-C21	-H43	: -51.563487
C23	-P17	-C21	-H44	:-172.208759
C23	-P17	-C21	-H45	: 70.261544
C23	-P17	-C22	-H46	: 171.405823
C23	-P17	-C22	-H47	: 51.248720
C23	-P17	-C22	-H49	: -71.453841
C23	-C24	-C25	-C26	: 0.474263
C23	-C24	-C25	-H48	: 179.967096
C23	-C28	-C27	-C26	: -0.088492
C23	-C28	-C27	-H52	: 179.749219
C24	-C23	-C28	-C27	: 0.450760
C24	-C23	-C28	-H51	:-179.254950
C24	-C25	-C26	-C27	: -0.093054
C24	-C25	-C26	-S29	:-179.886703
C25	-C24	-C23	-C28	: -0.642319
C25	-C26	-C27	-C28	: -0.097623
C25	-C26	-C27	-H52	:-179.931710
C25	-C26	-S29	-C30	:-174.102375
C26	-C25	-C24	-H50	:-178.435303
C26	-C27	-C28	-H51	: 179.623602

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C26     -S29     -C30     -H53     :  58.752718
C26     -S29     -C30     -H54     : 176.880855
C26     -S29     -C30     -H55     : -64.989847
C27     -C26     -C25     -H48     :-179.584723
C27     -C26     -S29     -C30     :   6.118118
C28     -C23     -C24     -H50     : 178.252723
C28     -C27     -C26     -S29     : 179.678087
S29     -C26     -C25     -H48     :   0.621628
S29     -C26     -C27     -H52     :  -0.156001
C31     -P18     -C32     -H59     :  50.242502
C31     -P18     -C32     -H60     : -70.346876
C31     -P18     -C32     -H61     : 171.464103
C31     -P18     -C33     -H56     :  68.603497
C31     -P18     -C33     -H57     :-173.641444
C31     -P18     -C33     -H58     : -52.425388
C32     -P18     -C31     -H62     : -50.018858
C32     -P18     -C31     -H63     :  70.696972
C32     -P18     -C31     -H64     :-171.210460
C32     -P18     -C33     -H56     : 173.185333
C32     -P18     -C33     -H57     : -69.059608
C32     -P18     -C33     -H58     :  52.156449
C33     -P18     -C31     -H62     :  55.057695
C33     -P18     -C31     -H63     : 175.773526
C33     -P18     -C31     -H64     : -66.133907
C33     -P18     -C32     -H59     : -54.886426
C33     -P18     -C32     -H60     :-175.475805
C33     -P18     -C32     -H61     :  66.335174
C34     -P19     -C35     -H71     :  52.493761
C34     -P19     -C35     -H72     : -68.550789
C34     -P19     -C35     -H73     : 173.482182
C34     -P19     -C36     -H68     : -50.804255
C34     -P19     -C36     -H69     :  69.841345
C34     -P19     -C36     -H70     :-171.927031
C35     -P19     -C34     -H65     :  66.867450
C35     -P19     -C34     -H66     :-174.956081
C35     -P19     -C34     -H67     : -54.350260
C35     -P19     -C36     -H68     :  54.175313
C35     -P19     -C36     -H69     : 174.820912
C35     -P19     -C36     -H70     : -66.947463
C36     -P19     -C34     -H65     : 171.660124
C36     -P19     -C34     -H66     : -70.163406
C36     -P19     -C34     -H67     :  50.442415
C36     -P19     -C35     -H71     : -52.085181
C36     -P19     -C35     -H72     :-173.129732
C36     -P19     -C35     -H73     :  68.903239
C37     -P15     -C38     -H86     :-171.594277
C37     -P15     -C38     -H87     : -50.275422
C37     -P15     -C38     -H88     :  70.401892
C37     -P15     -C39     -H80     : 172.829197
C37     -P15     -C39     -H81     :  51.645479
C37     -P15     -C39     -H82     : -69.292713
C38     -P15     -C37     -H83     : 171.646559
C38     -P15     -C37     -H84     :  50.539520
C38     -P15     -C37     -H85     : -70.136550
C38     -P15     -C39     -H80     :  68.133152
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C38     -P15     -C39     -H81     : -53.050567
C38     -P15     -C39     -H82     :-173.988758
C39     -P15     -C37     -H83     :  66.469627
C39     -P15     -C37     -H84     : -54.637412
C39     -P15     -C37     -H85     :-175.313482
C39     -P15     -C38     -H86     : -66.688457
C39     -P15     -C38     -H87     :  54.630398
C39     -P15     -C38     -H88     : 175.307711
C40     -P16     -C41     -H77     :-174.827225
C40     -P16     -C41     -H78     : -54.155076
C40     -P16     -C41     -H79     :  67.154008
C40     -P16     -C42     -H74     : 174.809646
C40     -P16     -C42     -H75     : -67.027215
C40     -P16     -C42     -H76     :  54.160329
C41     -P16     -C40     -H89     : -68.515013
C41     -P16     -C40     -H90     : 173.543957
C41     -P16     -C40     -H91     :  52.567485
C41     -P16     -C42     -H74     :  69.708609
C41     -P16     -C42     -H75     :-172.128252
C41     -P16     -C42     -H76     : -50.940708
C42     -P16     -C40     -H89     :-173.219618
C42     -P16     -C40     -H90     :  68.839351
C42     -P16     -C40     -H91     : -52.137120
C42     -P16     -C41     -H77     : -69.987931
C42     -P16     -C41     -H78     :  50.684218
C42     -P16     -C41     -H79     : 171.993302
H48     -C25     -C24     -H50     :   1.057530
H51     -C28     -C27     -H52     :  -0.538686
C92     -P20     -C93     -H102    : 171.642654
C92     -P20     -C93     -H103    :  51.411723
C92     -P20     -C93     -H104    : -70.994959
C92     -P20     -C94     -H105    :-173.716907
C92     -P20     -C94     -H106    :  68.720446
C92     -P20     -C94     -H107    : -53.236277
C92     -C95     -C96     -C97     :  -0.067316
C92     -C95     -C96     -H109    : 179.769784
C92     -C99     -C98     -C97     :   0.573169
C92     -C99     -C98     -H110    : 179.813579
C93     -P20     -C92     -C95     :  28.546720
C93     -P20     -C92     -C99     :-154.047049
C93     -P20     -C94     -H105    : -67.508491
C93     -P20     -C94     -H106    : 174.928863
C93     -P20     -C94     -H107    :  52.972139
C94     -P20     -C92     -C95     : 132.775303
C94     -P20     -C92     -C99     : -49.818465
C94     -P20     -C93     -H102    :  65.950105
C94     -P20     -C93     -H103    : -54.280825
C94     -P20     -C93     -H104    :-176.687508
C95     -C92     -C99     -C98     :  -0.584496
C95     -C92     -C99     -H111    : 178.262863
C95     -C96     -C97     -C98     :   0.037880
C95     -C96     -C97     -S100    : 179.935571
C96     -C95     -C92     -C99     :   0.332733
C96     -C97     -C98     -C99     :  -0.287952
C96     -C97     -C98     -H110    :-179.526719
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C96     -C97     -S100    -C101    :   6.159493
C97     -C96     -C95     -H108    : 179.568221
C97     -C98     -C99     -H111    :-178.289110
C97     -S100    -C101    -H112    :  58.259658
C97     -S100    -C101    -H113    : 176.358165
C97     -S100    -C101    -H114    : -65.451806
C98     -C97     -C96     -H109    :-179.795609
C98     -C97     -S100    -C101    :-173.941061
C99     -C92     -C95     -H108    :-179.294673
C99     -C98     -C97     -S100    : 179.806230
S100    -C97     -C96     -H109    :   0.102081
S100    -C97     -C98     -H110    :   0.567463
H108    -C95     -C96     -H109    :  -0.594679
H110    -C98     -C99     -H111    :   0.951300
```

co6se8_pme3_4_bis_3-thiomethylphenyl-dimethylphosphine

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 Energy components, in hartrees:
   (A)  Nuclear repulsion.............   12491.43638089661
   (E)  Total one-electron terms.....  -32134.85960675078
   (I)  Total two-electron terms.....   14673.34788149562
   (J)    Coulomb....................   15156.78978834750
   (K)    Exchange+Correlation.......    -483.44190685188
   (L)  Electronic energy............  -17461.51172525516  (E+I)
   (N)  Total energy.................   -4970.07534435855  (A+L)

 SCFE: SCF energy: DFT(b3lyp)     -4970.07534435855 hartrees


 HOMO energy:    -0.15745
 LUMO energy:    -0.05701

  Orbital energies (hartrees):
   -88.86232   -88.86188   -77.09504   -77.09423   -77.08988   -77.08977
   -77.08882   -77.08869   -10.21682   -10.21626   -10.21262   -10.21226
   -10.19152   -10.19080   -10.18815   -10.18753   -10.18748   -10.18682
   -10.18655   -10.18616   -10.18328   -10.17990   -10.17523   -10.17296
   -10.17262   -10.17254   -10.17244   -10.17240   -10.17180   -10.17118
   -10.17117   -10.17099   -10.17065   -10.17012   -10.16992   -10.16976
   -10.16944   -10.16904    -7.93828    -7.93780    -6.57184    -6.57107
    -6.56710    -6.56699    -6.56602    -6.56590    -5.90281    -5.90233
    -5.89867    -5.89818    -5.89228    -5.89180    -4.73388    -4.73360
    -4.73310    -4.73283    -4.73063    -4.72987    -4.72893    -4.72890
    -4.72883    -4.72880    -4.72785    -4.72782    -4.72774    -4.72770
    -4.72601    -4.72590    -4.72495    -4.72482    -3.70102    -3.70064
    -3.70003    -3.69935    -3.69922    -3.69919    -2.39517    -2.39491
    -2.39483    -2.39364    -2.39359    -2.39357    -2.39165    -2.39143
    -2.39141    -2.39078    -2.39049    -2.39046    -2.39028    -2.38999
    -2.38991    -2.38944    -2.38931    -2.38907    -0.86060    -0.86037
    -0.79874    -0.79866    -0.76558    -0.76506    -0.76276    -0.76256
    -0.76150    -0.76117    -0.74003    -0.73929    -0.72457    -0.72392
    -0.68877    -0.68789    -0.68689    -0.68668    -0.68557    -0.68552
    -0.68533    -0.68509    -0.68434    -0.68393    -0.65190    -0.65151
    -0.64289    -0.61537    -0.61400    -0.61361    -0.61013    -0.60896
    -0.59204    -0.59186    -0.59018    -0.58572    -0.58297    -0.57856
    -0.53757    -0.53636    -0.53594    -0.53538    -0.53478    -0.53413
    -0.50632    -0.50570    -0.45910    -0.45862    -0.44641    -0.44590
    -0.43852    -0.43804    -0.43675    -0.43630    -0.43543    -0.43532
    -0.43440    -0.43386    -0.42819    -0.42592    -0.42561    -0.42406
    -0.42080    -0.42068    -0.42054    -0.42024    -0.41967    -0.41928
    -0.41879    -0.41860    -0.40258    -0.40129    -0.40005    -0.39878
    -0.39852    -0.39817    -0.39733    -0.39717    -0.39687    -0.39675
    -0.39632    -0.39466    -0.38831    -0.38810    -0.38211    -0.38093
    -0.38015    -0.37986    -0.37856    -0.37839    -0.37043    -0.37037
    -0.35990    -0.35918    -0.33665    -0.33581    -0.33236    -0.33080
    -0.33060    -0.33022    -0.32997    -0.32964    -0.32922    -0.32887
    -0.32847    -0.32798    -0.32554    -0.32390    -0.31725    -0.31552
    -0.31514    -0.31024    -0.30736    -0.30694    -0.29121    -0.28972
    -0.28328    -0.28215    -0.28153    -0.27948    -0.27905    -0.27852
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-0.27739	-0.27712	-0.27638	-0.27595	-0.27484	-0.27369
-0.25301	-0.25266	-0.25221	-0.24593	-0.24459	-0.23680
-0.23548	-0.23477	-0.23431	-0.23030	-0.22974	-0.22801
-0.22729	-0.22714	-0.22526	-0.22498	-0.22458	-0.21942
-0.21420	-0.21386	-0.20625	-0.20591	-0.19657	-0.19614
-0.19490	-0.19057	-0.18937	-0.18901	-0.17994	-0.17934
-0.17844	-0.16913	-0.15926	-0.15830	-0.15745	-0.05701
-0.05154	-0.05123	-0.04658	-0.04284	-0.03494	-0.03429
-0.03322	-0.03077	-0.02995			

final geometry:

		angstroms	
atom	x	y	z
C1	-0.7228510235	0.0839616303	-0.2456560131
C2	-0.1977431308	-0.0287547239	1.0527463797
C3	1.1878353672	-0.0494468784	1.2192113300
C4	2.0534713703	0.0442571109	0.1175376213
C5	1.5209885829	0.1614742011	-1.1690125294
C6	0.1344507007	0.1798603654	-1.3360020786
P7	-1.3561741940	-0.1523995023	2.4888394721
C8	-2.3827308657	1.3671333900	2.2568825457
H9	2.1640031878	0.2391310014	-2.0383589485
Co10	-2.4830286861	-2.0174866880	2.7389585954
Se11	-0.9705382153	-3.5718726359	1.6800027796
Co12	-3.1617208018	-4.2556256745	0.9270542404
P13	-2.5950930506	-4.7973072712	-1.1108074495
C14	-3.7843536206	-5.8724376916	-2.0230004408
Co15	-4.0054214214	-3.3367869158	4.9164241882
P16	-4.3329815796	-2.8280564035	7.0155313693
C17	-3.8501835087	-1.1196874255	7.5201283331
Co18	-1.8925722687	-4.8333948709	3.5297796352
P19	-0.1714035107	-5.9552697339	4.2730259803
C20	1.4434389392	-5.6549544479	3.4333985698
Co21	-5.3075285106	-2.7542345796	2.3280250843
P22	-7.0474606842	-1.6175481422	1.6603233979
C23	-8.5850170018	-1.7666552851	2.6682697014
Se24	-3.7532701185	-1.9183342778	0.6808067172
Se25	-4.4242757235	-1.1703342117	3.9277850910
Se26	-1.6406976028	-2.8332427829	4.8623047373
Co27	-4.7191796298	-5.5640052378	3.0702928136
P28	-5.9054091125	-7.4024419795	3.0438215103
C29	-5.5128359643	-8.6910757971	4.3028112026
C30	-5.8989550821	-8.4870532199	5.6299326650
C31	-5.6099958967	-9.4333330118	6.6210259462
C32	-4.9113549761	-10.5951203123	6.2750553953
C33	-4.5123309855	-10.7928433314	4.9546182157
C34	-4.8070094146	-9.8557746873	3.9674526996
H35	-4.6706607776	-11.3457831166	7.0194287013
Se36	-3.4838820630	-5.6842040167	5.1393617673
Se37	-6.2066949030	-4.0167023329	4.1836188703
Se38	-2.7645669452	-6.4214256892	1.9258474961
Se39	-5.5433438225	-4.7293571454	0.9555142219
C40	-6.8318186366	0.2122742316	1.5691573196
C41	-7.6618730003	-1.9967671085	-0.0376763953
C42	-2.3375691743	-3.4052512523	-2.2929791787

C43	-1.0209606211	-5.7425532030	-1.2999391820
C44	-7.7256745819	-7.1750818913	3.2678928225
C45	-5.8709532602	-8.3493021088	1.4598487440
C46	-0.3084400332	-7.7933734710	4.1997811866
C47	0.2699692881	-5.6914828370	6.0453797960
C48	-3.4231450671	-3.8469211414	8.2550225202
C49	-6.0673963584	-2.9281816226	7.6358006459
C50	-0.3134484644	0.3476180714	3.9253019022
H51	-8.2498964142	-8.1335941081	3.1963957598
H52	-8.0789651805	-6.4959668410	2.4878809820
H53	-7.9312032069	-6.7104509674	4.2332252403
H54	-6.2841621774	-7.7045237321	0.6812827992
H55	-6.4629377406	-9.2667458441	1.5372570483
S56	-6.1734100595	-9.0538612690	8.2733280538
H57	-4.8417516121	-8.5879609322	1.1866816013
H58	-6.4134530991	-7.5707831914	5.9063598818
H59	-4.4803953362	-10.0339313787	2.9490429791
H60	-3.9658450670	-11.6962738032	4.6949400362
H61	1.3545374083	-5.9021986186	2.3731459318
H62	1.7006917759	-4.5959211516	3.5089701840
H63	2.2357555100	-6.2602601396	3.8882285209
H64	1.1162273197	-6.3264068495	6.3306253381
H65	-0.5952465613	-5.9324816976	6.6673904605
H66	0.5256231896	-4.6419980616	6.2052040288
H67	0.5718555958	-8.2651644339	4.6508983639
H68	-1.2089976918	-8.1056520016	4.7339139720
H69	-0.4052546200	-8.1100614254	3.1593307334
H70	-3.7360483394	-4.8895754553	8.1711004709
H71	-2.3528379042	-3.7930511551	8.0421001227
H72	-3.6145757331	-3.4826298962	9.2705521110
H73	-4.0245567995	-0.9691284960	8.5913576323
H74	-2.7916436101	-0.9688401745	7.2957009919
H75	-4.4279711805	-0.3932233009	6.9451538907
H76	-6.1187565242	-2.6392068008	8.6916047176
H77	-6.4387996620	-3.9482024791	7.5151209913
H78	-6.7027555954	-2.2669220889	7.0420870390
H79	-3.9376509752	-6.7938019744	-1.4561279577
H80	-4.7468281994	-5.3634273451	-2.1061746166
H81	-3.4043214442	-6.1148376713	-3.0217171840
H82	-1.0817217611	-6.6612392033	-0.7123080964
H83	-0.8421276640	-5.9877135597	-2.3528639982
H84	-0.1929099502	-5.1434700177	-0.9148435986
H85	-8.9024125807	-2.8113437709	2.6954845377
H86	-9.3860585673	-1.1470249548	2.2495597459
H87	-8.3756653939	-1.4538821169	3.6938166172
H88	-6.5981344141	0.6006565142	2.5623310020
H89	-7.7406314671	0.6905482246	1.1874120184
H90	-5.9924118331	0.4383007193	0.9075910352
H91	-7.9806439166	-3.0399068152	-0.0863646580
H92	-8.4975042206	-1.3398741004	-0.3039251703
H93	-6.8443994600	-1.8591850777	-0.7495057739
H94	-1.5810837948	-2.7282555795	-1.8887566678
H95	-3.2684246326	-2.8446782166	-2.4036735592
H96	-2.0130085368	-3.7811309180	-3.2699701986
H97	-0.9759777736	0.4699422581	4.7853764775

H98	0.2136302179	1.2863734278	3.7269592503
H99	0.3998117925	-0.4404825926	4.1723030519
H100	-3.0184468191	1.4908847301	3.1363512048
H101	-3.0303781371	1.2437939839	1.3869874048
H102	-1.7473270591	2.2482645957	2.1221756659
H103	1.6195470760	-0.1474977285	2.2103759444
S104	3.8015717763	0.0183805284	0.4869126078
H105	-0.2781005611	0.2718510873	-2.3379386413
H106	-1.7962794261	0.0721825301	-0.4038722822
C107	4.5832381962	0.0589362088	-1.1570725026
H108	5.6589451058	0.0142054146	-0.9727963555
H109	4.2912174914	-0.8054612588	-1.7581356425
H110	4.3555322965	0.9844902173	-1.6916747518
C111	-5.5562638830	-10.4523074892	9.2635818463
H112	-5.8639506444	-10.2432738458	10.2906412643
H113	-6.0018069568	-11.3995401182	8.9486476735
H114	-4.4660979509	-10.5187490329	9.2279880894

bond lengths (angstroms):

C1	-C2	:	1.405095	C1	-C6	:	1.390330
C1	-H106	:	1.085090	C2	-C3	:	1.395696
C2	-P7	:	1.849220	C3	-C4	:	1.404205
C3	-H103	:	1.085540	C4	-C5	:	1.397315
C4	-S104	:	1.786886	C5	-C6	:	1.396679
C5	-H9	:	1.084095	C6	-H105	:	1.087445
P7	-C8	:	1.848405	P7	-Co10	:	2.193379
P7	-C50	:	1.844104	C8	-H100	:	1.092206
C8	-H101	:	1.091502	C8	-H102	:	1.094658
Co10	-Se11	:	2.413531	Co10	-Se24	:	2.420606
Co10	-Se25	:	2.428871	Co10	-Se26	:	2.425609
Se11	-Co12	:	2.415726	Se11	-Co18	:	2.421417
Co12	-P13	:	2.183430	Co12	-Se24	:	2.423530
Co12	-Se38	:	2.417852	Co12	-Se39	:	2.428448
P13	-C14	:	1.844544	P13	-C42	:	1.844361
P13	-C43	:	1.845848	C14	-H79	:	1.092592
C14	-H80	:	1.091955	C14	-H81	:	1.095727
Co15	-P16	:	2.184572	Co15	-Se25	:	2.417925
Co15	-Se26	:	2.418347	Co15	-Se36	:	2.414968
Co15	-Se37	:	2.417621	P16	-C17	:	1.845599
P16	-C48	:	1.844512	P16	-C49	:	1.844710
C17	-H73	:	1.095722	C17	-H74	:	1.092533
C17	-H75	:	1.091872	Co18	-P19	:	2.184820
Co18	-Se26	:	2.416541	Co18	-Se36	:	2.418036
Co18	-Se38	:	2.419672	P19	-C20	:	1.844690
P19	-C46	:	1.844660	P19	-C47	:	1.845435
C20	-H61	:	1.092323	C20	-H62	:	1.092448
C20	-H63	:	1.095916	Co21	-P22	:	2.182944
Co21	-Se24	:	2.414079	Co21	-Se25	:	2.418286
Co21	-Se37	:	2.417758	Co21	-Se39	:	2.416713
P22	-C23	:	1.844524	P22	-C40	:	1.844739
P22	-C41	:	1.845132	C23	-H85	:	1.092179
C23	-H86	:	1.095868	C23	-H87	:	1.092429
Co27	-P28	:	2.188079	Co27	-Se36	:	2.412769

Co27	-Se37	:	2.417921	Co27	-Se38	:	2.421866
Co27	-Se39	:	2.418300	P28	-C29	:	1.843840
P28	-C44	:	1.848044	P28	-C45	:	1.845725
C29	-C30	:	1.397127	C29	-C34	:	1.402562
C30	-C31	:	1.400432	C30	-H58	:	1.086587
C31	-C32	:	1.399123	C31	-S56	:	1.786487
C32	-C33	:	1.393510	C32	-H35	:	1.084214
C33	-C34	:	1.392634	C33	-H60	:	1.087321
C34	-H59	:	1.084239	C40	-H88	:	1.091716
C40	-H89	:	1.095635	C40	-H90	:	1.092411
C41	-H91	:	1.091845	C41	-H92	:	1.095754
C41	-H93	:	1.092654	C42	-H94	:	1.092698
C42	-H95	:	1.092240	C42	-H96	:	1.095964
C43	-H82	:	1.092239	C43	-H83	:	1.095781
C43	-H84	:	1.092185	C44	-H51	:	1.094836
C44	-H52	:	1.092900	C44	-H53	:	1.090867
C45	-H54	:	1.092083	C45	-H55	:	1.094596
C45	-H57	:	1.091254	C46	-H67	:	1.095908
C46	-H68	:	1.092621	C46	-H69	:	1.091880
C47	-H64	:	1.095740	C47	-H65	:	1.092509
C47	-H66	:	1.091935	C48	-H70	:	1.091824
C48	-H71	:	1.092609	C48	-H72	:	1.095744
C49	-H76	:	1.095841	C49	-H77	:	1.092221
C49	-H78	:	1.092447	C50	-H97	:	1.092537
C50	-H98	:	1.094721	C50	-H99	:	1.091262
S56	-C111	:	1.821297	S104	-C107	:	1.820806
C107	-H108	:	1.092293	C107	-H109	:	1.092582
C107	-H110	:	1.092840	C111	-H112	:	1.092345
C111	-H113	:	1.093134	C111	-H114	:	1.092769

bond angles:

C6	-C1	-C2	: 119.985389	H106	-C1	-C2	: 120.236312
H106	-C1	-C6	: 119.761492	C3	-C2	-C1	: 118.842987
P7	-C2	-C1	: 119.266762	P7	-C2	-C3	: 121.889739
C4	-C3	-C2	: 121.159891	H103	-C3	-C2	: 120.334709
H103	-C3	-C4	: 118.503419	C5	-C4	-C3	: 119.540725
S104	-C4	-C3	: 116.099694	S104	-C4	-C5	: 124.356964
C6	-C5	-C4	: 119.307558	H9	-C5	-C4	: 121.219795
H9	-C5	-C6	: 119.472626	C5	-C6	-C1	: 121.162549
H105	-C6	-C1	: 119.635039	H105	-C6	-C5	: 119.202388
C8	-P7	-C2	: 101.273266	Co10	-P7	-C2	: 117.855957
Co10	-P7	-C8	: 115.341917	C50	-P7	-C2	: 103.449186

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 C50     -P7     -C8     : 100.887347  C50     -P7     -Co10    :
115.609134
 H100    -C8     -P7     : 108.382025  H101    -C8     -P7      :
109.672969
 H101    -C8     -H100   : 108.009906  H102    -C8     -P7      :
110.780693
 H102    -C8     -H100   : 110.227056  H102    -C8     -H101    :
109.712539
 Se11    -Co10   -P7     : 100.116374  Se24    -Co10   -P7      :
97.921039
 Se24    -Co10   -Se11   :  88.978596  Se25    -Co10   -P7      :
99.778805
 Se25    -Co10   -Se11   : 160.091935  Se25    -Co10   -Se24    :
88.995560
 Se26    -Co10   -P7     : 101.969316  Se26    -Co10   -Se11    :
87.126434
 Se26    -Co10   -Se24   : 160.104823  Se26    -Co10   -Se25    :
88.073589
 Co12    -Se11   -Co10   :  75.559222  Co18    -Se11   -Co10    :
76.215358
 Co18    -Se11   -Co12   :  75.241501  P13     -Co12   -Se11    :
97.223190
 Se24    -Co12   -Se11   :  88.859547  Se24    -Co12   -P13     :
101.991701
 Se38    -Co12   -Se11   :  88.612765  Se38    -Co12   -P13     :
96.932387
 Se38    -Co12   -Se24   : 161.075257  Se39    -Co12   -Se11    :
160.240805
 Se39    -Co12   -P13    : 102.535884  Se39    -Co12   -Se24    :
87.130898
 Se39    -Co12   -Se38   :  88.940579  C14     -P13    -Co12    :
116.030447
 C42     -P13    -Co12   : 116.565486  C42     -P13    -C14     :
102.296647
 C43     -P13    -Co12   : 116.358581  C43     -P13    -C14     :
101.576756
 C43     -P13    -C42    : 101.639875  H79     -C14    -P13     :
108.990132
 H80     -C14    -P13    : 109.527497  H80     -C14    -H79     :
107.995557
 H81     -C14    -P13    : 110.859578  H81     -C14    -H79     :
109.572959
 H81     -C14    -H80    : 109.840373  Se25    -Co15   -P16     :
99.105571
 Se26    -Co15   -P16    :  96.870879  Se26    -Co15   -Se25    :
88.491494
 Se36    -Co15   -P16    :  99.790070  Se36    -Co15   -Se25    :
161.100845
 Se36    -Co15   -Se26   :  89.615393  Se37    -Co15   -P16     :
102.721915
 Se37    -Co15   -Se25   :  88.299309  Se37    -Co15   -Se26    :
160.406816
 Se37    -Co15   -Se36   :  87.205737  C17     -P16    -Co15    :
116.042905
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 C48     -P16     -Co15    : 116.302048  C48     -P16     -C17     :
101.451769
 C49     -P16     -Co15    : 116.835184  C49     -P16     -C17     :
101.786431
 C49     -P16     -C48     : 101.995926  H73     -C17     -P16     :
110.661932
 H74     -C17     -P16     : 108.971443  H74     -C17     -H73     :
109.636051
 H75     -C17     -P16     : 109.479191  H75     -C17     -H73     :
109.827546
 H75     -C17     -H74     : 108.220216  P19     -Co18    -Se11    :
103.145222
 Se26    -Co18    -Se11    :  87.153363  Se26    -Co18    -P19     :
98.934946
 Se36    -Co18    -Se11    : 160.461621  Se36    -Co18    -P19     :
96.391354
 Se36    -Co18    -Se26    :  89.585715  Se38    -Co18    -Se11    :
88.439349
 Se38    -Co18    -P19     :  99.927320  Se38    -Co18    -Se26    :
161.137226
 Se38    -Co18    -Se36    :  88.461729  C20     -P19     -Co18    :
116.820253
 C46     -P19     -Co18    : 116.080302  C46     -P19     -C20     :
102.074335
 C47     -P19     -Co18    : 116.214405  C47     -P19     -C20     :
101.799885
 C47     -P19     -C46     : 101.439535  H61     -C20     -P19     :
109.493498
 H62     -C20     -P19     : 109.419134  H62     -C20     -H61     :
107.802379
 H63     -C20     -P19     : 110.736452  H63     -C20     -H61     :
109.673567
 H63     -C20     -H62     : 109.662406  Se24    -Co21    -P22     :
97.132237
 Se25    -Co21    -P22     :  98.766554  Se25    -Co21    -Se24    :
89.395110
 Se37    -Co21    -P22     : 102.135456  Se37    -Co21    -Se24    :
160.722543
 Se37    -Co21    -Se25    :  88.287874  Se39    -Co21    -P22     :
100.025088
 Se39    -Co21    -Se24    :  87.609895  Se39    -Co21    -Se25    :
161.195835
 Se39    -Co21    -Se37    :  88.443199  C23     -P22     -Co21    :
117.076025
 C40     -P22     -Co21    : 116.004736  C40     -P22     -C23     :
101.807917
 C41     -P22     -Co21    : 116.095944  C41     -P22     -C23     :
102.045616
 C41     -P22     -C40     : 101.379616  H85     -C23     -P22     :
109.462127
 H86     -C23     -P22     : 110.782437  H86     -C23     -H85     :
109.751097
 H87     -C23     -P22     : 109.275274  H87     -C23     -H85     :
107.827946
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H87 -C23 -H86 : 109.687079 Co12 -Se24 -Co10 :
75.286625
Co21 -Se24 -Co10 : 75.137948 Co21 -Se24 -Co12 :
75.751994
Co15 -Se25 -Co10 : 75.473234 Co21 -Se25 -Co10 :
74.911078
Co21 -Se25 -Co15 : 75.339270 Co15 -Se26 -Co10 :
75.525458
Co18 -Se26 -Co10 : 76.081665 Co18 -Se26 -Co15 :
74.816050
Se36 -Co27 -P28 : 104.245690 Se37 -Co27 -P28 :
102.106054
Se37 -Co27 -Se36 : 87.248608 Se38 -Co27 -P28 :
97.721676
Se38 -Co27 -Se36 : 88.532462 Se38 -Co27 -Se37 :
160.161328
Se39 -Co27 -P28 : 95.431012 Se39 -Co27 -Se36 :
160.321682
Se39 -Co27 -Se37 : 88.402871 Se39 -Co27 -Se38 :
89.083487
C29 -P28 -Co27 : 117.614581 C44 -P28 -Co27 :
115.413540
C44 -P28 -C29 : 102.292553 C45 -P28 -Co27 :
115.549377
C45 -P28 -C29 : 102.913012 C45 -P28 -C44 :
100.693410
C30 -C29 -P28 : 119.189218 C34 -C29 -P28 :
121.617331
C34 -C29 -C30 : 119.174225 C31 -C30 -C29 :
121.100912
H58 -C30 -C29 : 119.712772 H58 -C30 -C31 :
119.173266
C32 -C31 -C30 : 119.282610 S56 -C31 -C30 :
116.483981
S56 -C31 -C32 : 124.233313 C33 -C32 -C31 :
119.677257
H35 -C32 -C31 : 121.063997 H35 -C32 -C33 :
119.258371
C34 -C33 -C32 : 121.038530 H60 -C33 -C32 :
119.216367
H60 -C33 -C34 : 119.744684 C33 -C34 -C29 :
119.719695
H59 -C34 -C29 : 120.839222 H59 -C34 -C33 :
119.439577
Co18 -Se36 -Co15 : 74.850210 Co27 -Se36 -Co15 :
76.222185
Co27 -Se36 -Co18 : 75.438073 Co21 -Se37 -Co15 :
75.354498
Co27 -Se37 -Co15 : 76.077178 Co27 -Se37 -Co21 :
75.638889
Co18 -Se38 -Co12 : 75.234620 Co27 -Se38 -Co12 :
75.256651
Co27 -Se38 -Co18 : 75.241788 Co21 -Se39 -Co12 :
75.612978

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 Co27    -Se39    -Co12    :  75.128314  Co27    -Se39    -Co21    :
75.651136
 H88     -C40     -P22     : 109.447347  H89     -C40     -P22     :
110.686390
 H89     -C40     -H88     : 109.830019  H90     -C40     -P22     :
108.964607
 H90     -C40     -H88     : 108.231263  H90     -C40     -H89     :
109.636323
 H91     -C41     -P22     : 109.548912  H92     -C41     -P22     :
110.752934
 H92     -C41     -H91     : 109.832030  H93     -C41     -P22     :
108.936037
 H93     -C41     -H91     : 108.039709  H93     -C41     -H92     :
109.680111
 H94     -C42     -P13     : 109.097487  H95     -C42     -P13     :
109.471116
 H95     -C42     -H94     : 108.030798  H96     -C42     -P13     :
110.724553
 H96     -C42     -H94     : 109.708860  H96     -C42     -H95     :
109.758887
 H82     -C43     -P13     : 109.156916  H83     -C43     -P13     :
110.622231
 H83     -C43     -H82     : 109.746688  H84     -C43     -P13     :
109.240615
 H84     -C43     -H82     : 108.290820  H84     -C43     -H83     :
109.742289
 H51     -C44     -P28     : 110.854088  H52     -C44     -P28     :
107.957592
 H52     -C44     -H51     : 110.036999  H53     -C44     -P28     :
110.198414
 H53     -C44     -H51     : 109.905511  H53     -C44     -H52     :
107.818630
 H54     -C45     -P28     : 107.569952  H55     -C45     -P28     :
111.050487
 H55     -C45     -H54     : 109.916097  H57     -C45     -P28     :
110.158906
 H57     -C45     -H54     : 107.909581  H57     -C45     -H55     :
110.149322
 H67     -C46     -P19     : 110.668177  H68     -C46     -P19     :
109.063158
 H68     -C46     -H67     : 109.742119  H69     -C46     -P19     :
109.477190
 H69     -C46     -H67     : 109.792182  H69     -C46     -H68     :
108.050316
 H64     -C47     -P19     : 110.603680  H65     -C47     -P19     :
109.017194
 H65     -C47     -H64     : 109.609301  H66     -C47     -P19     :
109.508800
 H66     -C47     -H64     : 109.754854  H66     -C47     -H65     :
108.306640
 H70     -C48     -P16     : 109.541185  H71     -C48     -P16     :
108.966179
 H71     -C48     -H70     : 108.230621  H72     -C48     -P16     :
110.669495
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 H72     -C48     -H70     : 109.795098  H72     -C48     -H71     :
109.594156
 H76     -C49     -P16     : 110.714450  H77     -C49     -P16     :
109.466188
 H77     -C49     -H76     : 109.681176  H78     -C49     -P16     :
109.343289
 H78     -C49     -H76     : 109.678282  H78     -C49     -H77     :
107.907004
 H97     -C50     -P7      : 107.498370  H98     -C50     -P7      :
111.323065
 H98     -C50     -H97     : 109.791032  H99     -C50     -P7      :
110.491524
 H99     -C50     -H97     : 107.399531  H99     -C50     -H98     :
110.219308
 C111    -S56     -C31     : 103.468344  C107    -S104    -C4      :
103.474708
 H108    -C107    -S104    : 105.637108  H109    -C107    -S104    :
111.367251
 H109    -C107    -H108    : 108.882525  H110    -C107    -S104    :
111.783201
 H110    -C107    -H108    : 108.808666  H110    -C107    -H109    :
110.196410
 H112    -C111    -S56     : 105.594845  H113    -C111    -S56     :
111.752262
 H113    -C111    -H112    : 108.777756  H114    -C111    -S56     :
111.531823
 H114    -C111    -H112    : 108.860496  H114    -C111    -H113    :
110.153869

  torsional angles:

 C1      -C2      -C3      -C4      :   0.203040
 C1      -C2      -C3      -H103    :-179.277297
 C1      -C2      -P7      -C8      : -55.462776
 C1      -C2      -P7      -Co10    :  71.334570
 C1      -C2      -P7      -C50     :-159.685632
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P28     -C29     -C34     -C33     : 178.926725
P28     -C29     -C34     -H59     :  -0.624442
C29     -P28     -Co27    -Se36    : -10.869650
C29     -P28     -Co27    -Se37    :-101.087666
C29     -P28     -Co27    -Se38    :  79.574962
C29     -P28     -Co27    -Se39    : 169.384539
C29     -P28     -C44     -H51     : -53.655282
C29     -P28     -C44     -H52     :-174.244974
C29     -P28     -C44     -H53     :  68.239448
C29     -P28     -C45     -H54     : 169.113484
C29     -P28     -C45     -H55     :  48.799996
C29     -P28     -C45     -H57     : -73.508645
C29     -C30     -C31     -C32     :   0.630823
C29     -C30     -C31     -S56     :-179.477345
C29     -C34     -C33     -C32     :   0.189765
C29     -C34     -C33     -H60     : 179.952361
C30     -C29     -P28     -C44     : -53.349488
C30     -C29     -P28     -C45     :-157.519058
C30     -C29     -C34     -C33     :   0.535036
C30     -C29     -C34     -H59     :-179.016131
C30     -C31     -C32     -C33     :   0.103609
C30     -C31     -C32     -H35     : 179.879192
C30     -C31     -S56     -C111    :-177.574812
C31     -C30     -C29     -C34     :  -0.949735
C31     -C32     -C33     -C34     :  -0.512270
C31     -C32     -C33     -H60     : 179.723900
C31     -S56     -C111    -H112    : 178.762531
C31     -S56     -C111    -H113    : -63.126033
C31     -S56     -C111    -H114    :  60.668383
C32     -C31     -C30     -H58     :-178.051146
C32     -C31     -S56     -C111    :   2.311072
C32     -C33     -C34     -H59     : 179.747254
C33     -C32     -C31     -S56     :-179.779287
C34     -C29     -P28     -C44     : 128.259058
C34     -C29     -P28     -C45     :  24.089488
C34     -C29     -C30     -H58     : 177.725209
C34     -C33     -C32     -H35     : 179.708074
H35     -C32     -C31     -S56     :  -0.003703
H35     -C32     -C33     -H60     :  -0.055756
Se36    -Co15    -P16     -C48     :  27.886340
Se36    -Co15    -P16     -C49     : -92.769721
Se36    -Co18    -P19     -C46     :  61.784741
Se36    -Co18    -P19     -C47     : -57.367666
Se36    -Co27    -P28     -C44     : 110.098292
Se36    -Co27    -P28     -C45     :-132.848109
Se37    -Co15    -P16     -C48     : 117.212543
Se37    -Co15    -P16     -C49     :  -3.443517
Se37    -Co21    -P22     -C40     : 125.254066
Se37    -Co21    -P22     -C41     :-115.838247
Se37    -Co27    -P28     -C44     :  19.880277
Se37    -Co27    -P28     -C45     : 136.933875
Se38    -Co12    -P13     -C42     :-166.664848
Se38    -Co12    -P13     -C43     : -46.697591
Se38    -Co18    -P19     -C46     : -27.767296
Se38    -Co18    -P19     -C47     :-146.919703
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Se38	-Co27	-P28	-C44	:-159.457096
Se38	-Co27	-P28	-C45	: -42.403497
Se39	-Co12	-P13	-C42	: 102.879376
Se39	-Co12	-P13	-C43	:-137.153366
Se39	-Co21	-P22	-C40	:-144.184848
Se39	-Co21	-P22	-C41	: -25.277161
Se39	-Co27	-P28	-C44	: -69.647519
Se39	-Co27	-P28	-C45	: 47.406080
C40	-P22	-C23	-H85	: 172.886167
C40	-P22	-C23	-H86	: 51.723623
C40	-P22	-C23	-H87	: -69.236812
C40	-P22	-C41	-H91	:-171.452216
C40	-P22	-C41	-H92	: -50.150501
C40	-P22	-C41	-H93	: 70.562725
C41	-P22	-C23	-H85	: 68.365908
C41	-P22	-C23	-H86	: -52.796636
C41	-P22	-C23	-H87	:-173.757071
C41	-P22	-C40	-H88	: 172.216842
C41	-P22	-C40	-H89	: 51.027223
C41	-P22	-C40	-H90	: -69.608693
C42	-P13	-C14	-H79	: 174.304904
C42	-P13	-C14	-H80	: -67.744137
C42	-P13	-C14	-H81	: 53.622831
C42	-P13	-C43	-H82	:-174.696010
C42	-P13	-C43	-H83	: -53.839694
C42	-P13	-C43	-H84	: 67.065293
C43	-P13	-C14	-H79	: 69.505447
C43	-P13	-C14	-H80	:-172.543594
C43	-P13	-C14	-H81	: -51.176625
C43	-P13	-C42	-H94	: -71.005985
C43	-P13	-C42	-H95	: 170.970370
C43	-P13	-C42	-H96	: 49.829374
C44	-P28	-C45	-H54	: 63.711996
C44	-P28	-C45	-H55	: -56.601492
C44	-P28	-C45	-H57	:-178.910133
C45	-P28	-C44	-H51	: 52.241410
C45	-P28	-C44	-H52	: -68.348281
C45	-P28	-C44	-H53	: 174.136141
C46	-P19	-C20	-H61	: 68.360765
C46	-P19	-C20	-H62	:-173.690499
C46	-P19	-C20	-H63	: -52.696148
C46	-P19	-C47	-H64	: 50.830496
C46	-P19	-C47	-H65	: -69.754216
C46	-P19	-C47	-H66	: 171.913635
C47	-P19	-C20	-H61	: 172.950002
C47	-P19	-C20	-H62	: -69.101262
C47	-P19	-C20	-H63	: 51.893088
C47	-P19	-C46	-H67	: -49.472069
C47	-P19	-C46	-H68	: 71.346921
C47	-P19	-C46	-H69	:-170.622388
C48	-P16	-C17	-H73	: -51.360325
C48	-P16	-C17	-H74	: 69.264410
C48	-P16	-C17	-H75	:-172.552029
C48	-P16	-C49	-H76	: 52.878014
C48	-P16	-C49	-H77	: -68.156413

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C48     -P16     -C49     -H78     : 173.828617
C49     -P16     -C17     -H73     :  53.644572
C49     -P16     -C17     -H74     : 174.269307
C49     -P16     -C17     -H75     : -67.547132
C49     -P16     -C48     -H70     :  66.677130
C49     -P16     -C48     -H71     :-175.093855
C49     -P16     -C48     -H72     : -54.519605
C50     -P7      -C8      -H100    : -65.368177
C50     -P7      -C8      -H101    : 176.934002
C50     -P7      -C8      -H102    :  55.681802
S56     -C31     -C30     -H58     :   1.840686
H59     -C34     -C33     -H60     :  -0.490150
H103    -C3      -C4      -S104    :  -1.019808
H105    -C6      -C1      -H106    :   1.790635
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co6se8_pme3_4_bis_monoenedimethylphosphine

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 Energy components, in hartrees:
   (A)  Nuclear repulsion.............   15350.76598511184
   (E)  Total one-electron terms.....  -38670.15812659328
   (I)  Total two-electron terms.....   17732.39744587848
   (J)    Coulomb....................   18307.25384741550
   (K)    Exchange+Correlation.......    -574.85640153702
   (L)  Electronic energy............  -20937.76068071480  (E+I)
   (N)  Total energy.................   -5586.99469560297  (A+L)

 SCFE: SCF energy: DFT(b3lyp)     -5586.99469560297 hartrees


 HOMO energy:    -0.15781
 LUMO energy:    -0.06250

  Orbital energies (hartrees):
   -88.86724   -88.86682   -77.09555   -77.09454   -77.09066   -77.09014
   -77.08914   -77.08890   -10.21990   -10.21971   -10.21614   -10.21586
   -10.19497   -10.19463   -10.19445   -10.19429   -10.19146   -10.19132
   -10.18954   -10.18949   -10.18945   -10.18934   -10.18878   -10.18858
   -10.18852   -10.18851   -10.18800   -10.18772   -10.18684   -10.18632
   -10.18606   -10.18540   -10.18455   -10.18449   -10.18437   -10.18349
   -10.18295   -10.18252   -10.17582   -10.17422   -10.17422   -10.17374
   -10.17330   -10.17300   -10.17263   -10.17181   -10.17175   -10.17163
   -10.17128   -10.17127   -10.17011   -10.16996   -10.16970   -10.16848
    -7.94319    -7.94279    -6.57227    -6.57143    -6.56787    -6.56729
    -6.56639    -6.56619    -5.90767    -5.90728    -5.90353    -5.90314
    -5.89728    -5.89688    -4.73426    -4.73410    -4.73340    -4.73324
    -4.73106    -4.73023    -4.72971    -4.72969    -4.72914    -4.72912
    -4.72822    -4.72818    -4.72804    -4.72796    -4.72676    -4.72619
    -4.72531    -4.72513    -3.70070    -3.70069    -3.70063    -3.70029
    -3.70024    -3.69925    -2.39539    -2.39494    -2.39486    -2.39466
    -2.39454    -2.39379    -2.39155    -2.39133    -2.39131    -2.39128
    -2.39109    -2.39080    -2.39072    -2.39071    -2.39036    -2.39016
    -2.38994    -2.38936    -0.86652    -0.86645    -0.85602    -0.85580
    -0.81354    -0.81353    -0.78951    -0.78935    -0.76364    -0.76315
    -0.76304    -0.76290    -0.76156    -0.76140    -0.74918    -0.74896
    -0.74321    -0.74318    -0.73971    -0.73956    -0.70738    -0.70708
    -0.68959    -0.68846    -0.68777    -0.68699    -0.68644    -0.68614
    -0.68567    -0.68560    -0.68453    -0.68398    -0.65796    -0.65790
    -0.64276    -0.62526    -0.62504    -0.61481    -0.61358    -0.61335
    -0.61058    -0.60996    -0.60306    -0.60260    -0.59237    -0.59154
    -0.58970    -0.58146    -0.58134    -0.57863    -0.55528    -0.55516
    -0.54882    -0.54830    -0.53706    -0.53623    -0.53480    -0.53460
    -0.50625    -0.50596    -0.49543    -0.49516    -0.46418    -0.46413
    -0.45928    -0.45908    -0.45136    -0.45120    -0.44453    -0.44436
    -0.43871    -0.43805    -0.43786    -0.43769    -0.43746    -0.43731
    -0.43620    -0.43521    -0.43037    -0.43009    -0.42686    -0.42651
    -0.42178    -0.42147    -0.42123    -0.42086    -0.42076    -0.42062
    -0.41996    -0.41970    -0.41905    -0.41840    -0.41726    -0.41716
    -0.40318    -0.40307    -0.40178    -0.40142    -0.39965    -0.39900
    -0.39818    -0.39784    -0.39765    -0.39719    -0.39558    -0.39529
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-0.39194	-0.39132	-0.38996	-0.38833	-0.38118	-0.38103
-0.38101	-0.38046	-0.37890	-0.37857	-0.37118	-0.37098
-0.36774	-0.36763	-0.35667	-0.35658	-0.34720	-0.34699
-0.33912	-0.33882	-0.33637	-0.33392	-0.33172	-0.33113
-0.33092	-0.33041	-0.32971	-0.32944	-0.32909	-0.32881
-0.32772	-0.32756	-0.32580	-0.32413	-0.32073	-0.32056
-0.31740	-0.31680	-0.31597	-0.30917	-0.30751	-0.30678
-0.29057	-0.28962	-0.28385	-0.28293	-0.28024	-0.27996
-0.27801	-0.27793	-0.27757	-0.27672	-0.27524	-0.27401
-0.27062	-0.26980	-0.25536	-0.25512	-0.25392	-0.25226
-0.25197	-0.24973	-0.24762	-0.23664	-0.23628	-0.23575
-0.23564	-0.23147	-0.23087	-0.23030	-0.22925	-0.22830
-0.22772	-0.22635	-0.22605	-0.22532	-0.22511	-0.22028
-0.21463	-0.21426	-0.19661	-0.19590	-0.19510	-0.19293
-0.19151	-0.19069	-0.18971	-0.18860	-0.18009	-0.17947
-0.17848	-0.16868	-0.16045	-0.15798	-0.15781	-0.06250
-0.05596	-0.05208	-0.05151	-0.04480	-0.04335	-0.04121
-0.03569	-0.03407	-0.03336			

final geometry:

		angstroms	
atom	x	y	z
C1	-1.5756438942	-0.8753181077	-1.3065133784
C2	-0.9397040386	-0.5024670923	-0.1089360267
C3	0.4641014471	-0.3959039944	-0.1413259673
C4	1.1934697440	-0.6372218008	-1.2972560165
C5	0.5408764095	-1.0032048609	-2.4841703833
C6	-0.8559616628	-1.1196906255	-2.4701018034
C7	-1.6507998632	-0.2085465903	1.1372275310
C8	-2.9887698125	-0.2117428030	1.3083754233
C9	-3.7537062097	0.1208040193	2.5084437342
C10	-5.1589755277	0.1347351254	2.4127663400
C11	-5.9609677236	0.4878271236	3.4882990417
C12	-5.3953985115	0.8314486993	4.7253172164
C13	-3.9973829929	0.8066948111	4.8344907619
C14	-3.1927213982	0.4603512171	3.7533289911
P15	-6.5079244509	1.3334572688	6.1067304229
C16	-7.8673287105	0.0877242427	5.9746296114
S17	1.5651237684	-1.2859949954	-3.9138648755
C18	0.3658495026	-1.6601788393	-5.2327636592
C19	-5.5959583415	0.7167150492	7.5887591217
Co20	-7.1371491279	3.4357061870	6.1903096858
Se21	-9.5626026857	3.3032479247	6.1566896387
Co22	-9.1153351806	5.1223527853	7.6846136511
Se23	-7.3076199594	3.7819816356	8.5802665736
Co24	-6.2200947320	5.7887452395	7.7827446009
Se25	-4.9168781143	4.3752502916	6.3090315077
Co26	-6.1288881511	5.8736179636	4.8395784379
Se27	-5.6785741124	7.6889995386	6.3736735898
Co28	-8.0969459892	7.5444975058	6.3323902315
Se29	-8.0678570526	7.0501343757	8.7087549671
Se30	-7.1841208485	3.9491027983	3.8204782045
Co31	-9.0204636306	5.2098411550	4.7469028712
P32	-10.4816226322	4.8089432281	3.1714871618

C33	-10.5026178381	3.0952101527	2.4872755625
Se34	-7.9332184775	7.2105367652	3.9432787117
Se35	-10.3221245332	6.6193872244	6.2140740004
P36	-4.4903726934	6.2304112134	3.4378311114
C37	-4.7550179784	7.5688271873	2.1956455218
C38	-2.8792298635	6.7272216731	4.1874562384
C39	-3.9897704846	4.8045439371	2.3820451233
P40	-4.7751202873	6.1788587432	9.3749634286
C41	-4.9815846160	5.2203145054	10.9378056581
C42	-4.7284591477	7.9126964181	10.0072716480
C43	-2.9978398399	5.8847180463	8.9777676025
P44	-8.5887939457	9.6719631420	6.4579726393
C45	-10.1904066338	10.1488469559	7.2173351748
P46	-10.7520818246	4.7501467762	9.0844257989
C47	-11.2191010942	6.1451111735	10.1966362921
C48	-10.4998835116	3.3643503336	10.2760209464
C49	-12.3785374277	4.3089341490	8.3329918072
C50	-7.3848478518	10.7134683052	7.3976052096
C51	-8.6257643092	10.5615143896	4.8398083887
C52	-10.3370942540	5.8189082326	1.6343705581
C53	-12.2548906270	5.0444848917	3.6234024690
H54	-7.7409504292	11.7452910840	7.4742056062
H55	-7.2240019047	10.3011438341	8.3956442889
H56	-6.4296844884	10.6797508405	6.8677381468
H57	-8.8900852527	11.6159535623	4.9703051306
H58	-7.6307215981	10.4769845794	4.3952591090
H59	-9.3251927692	10.0796101661	4.1555891023
H60	-11.3817913951	3.2310493691	10.9128862577
H61	-10.3070566060	2.4445594981	9.7186116386
H62	-9.6248974910	3.5709848501	10.8962694588
H63	-12.0891686654	5.8788394087	10.8076589438
H64	-10.3745774569	6.3909872953	10.8440088061
H65	-11.4488116106	7.0263944944	9.5929363995
H66	-13.1314075834	4.1426358990	9.1115641310
H67	-12.7011023761	5.1206417333	7.6771265313
H68	-12.2628511267	3.4047273355	7.7312762570
H69	-4.2348732763	5.5236514618	11.6802797457
H70	-5.9853719283	5.3921559723	11.3336437080
H71	-4.8824410179	4.1529621740	10.7286133127
H72	-3.9636891404	8.0216095950	10.7846283240
H73	-4.5112494012	8.5907571150	9.1788919167
H74	-5.7082351729	8.1716581493	10.4147128241
H75	-2.3612487091	6.1516451542	9.8287990466
H76	-2.8492179397	4.8341129978	8.7200191660
H77	-2.7213897855	6.4876234106	8.1095600859
H78	-12.9097542102	4.7863435710	2.7833726440
H79	-12.4906118986	4.4096825576	4.4808132172
H80	-12.4202591988	6.0829509617	3.9169594236
H81	-11.0929423135	5.5199617219	0.8992155088
H82	-10.4591145308	6.8760323021	1.8802179150
H83	-9.3388234312	5.6869948017	1.2104674061
H84	-11.2874339244	2.9933405847	1.7293644045
H85	-9.5300251082	2.8713009903	2.0437502137
H86	-10.6819970992	2.3871792139	3.2996965694
H87	-2.1242157826	6.8808558964	3.4085681223

H88	-3.0134795742	7.6479893729	4.7591853283
H89	-2.5463615494	5.9429823641	4.8711073800
H90	-3.8743499676	7.6845673108	1.5537411326
H91	-5.6284290918	7.3319776853	1.5842723279
H92	-4.9546044291	8.5076716380	2.7178942147
H93	-3.1133047612	5.0605194163	1.7761465661
H94	-3.7599565206	3.9465294088	3.0178321447
H95	-4.8201741760	4.5250383598	1.7300107753
H96	-8.4930471187	0.1663744232	6.8670124703
H97	-7.4625161988	-0.9257310017	5.8860525671
H98	-8.4988409682	0.3114338627	5.1135755837
H99	-6.2605342184	0.7751676024	8.4529931169
H100	-4.7377121247	1.3613826625	7.7897263680
H101	-5.2590925950	-0.3144417593	7.4408766889
H102	-7.0360152272	0.5209834184	3.3489938159
H103	-5.6246729479	-0.1187972102	1.4630934298
H104	-2.1135600960	0.4628979516	3.8805381087
H105	-3.5200178301	1.0760559635	5.7721285995
H106	-3.6123078305	-0.4638125192	0.4523419138
H107	-1.0111298828	0.0549361569	1.9790679702
H108	0.9926807886	-0.1101376528	0.7649608056
H109	2.2759884978	-0.5397946647	-1.2813835153
H110	-1.3957213910	-1.4024326933	-3.3672468565
H111	-2.6556275789	-0.9775431415	-1.3421346401
H112	0.9627115140	-1.8537291954	-6.1267206205
H113	-0.2216476516	-2.5523400194	-5.0020694587
H114	-0.2956525734	-0.8120131706	-5.4248670607
C115	-10.2845264368	10.3191563258	8.6050609965
C116	-11.4949118517	10.6574456318	9.1963496324
C117	-12.6666257954	10.8300305713	8.4376359948
C118	-12.5640478796	10.6566633765	7.0443224924
C119	-11.3535839627	10.3228019694	6.4516812235
H120	-9.4135932507	10.1631894992	9.2347205102
H121	-11.5444878429	10.7825628342	10.2760538865
C122	-13.9022514323	11.1566303657	9.1429851686
H123	-13.4398241844	10.7815809559	6.4144557336
H124	-11.3222889583	10.1857586295	5.3745900942
C125	-15.1376347666	11.2988750795	8.6219317695
H126	-13.7751961496	11.2732427985	10.2168074745
C127	-16.3644839878	11.5854926944	9.3628168731
H128	-15.2632072625	11.1766509735	7.5472522852
C129	-17.5842229882	11.6950840214	8.6668771764
C130	-18.7783410617	11.9425596994	9.3255194367
C131	-18.8027104746	12.0946118016	10.7209837447
C132	-17.5990779125	11.9962244176	11.4303270235
C133	-16.4066925858	11.7463248785	10.7601092058
H134	-17.5848773308	11.5759069306	7.5857456649
H135	-19.7044905376	12.0151473125	8.7606164702
S136	-20.3949804729	12.4038877540	11.4577825034
H137	-17.5804703971	12.1112736237	12.5089868357
H138	-15.4936865977	11.6710409769	11.3404114258
C139	-20.0458632887	12.4103289888	13.2462140116
H140	-21.0081519663	12.5757142308	13.7354347884
H141	-19.6417917113	11.4503672184	13.5753587493
H142	-19.3685757231	13.2224341971	13.5191314863

bond lengths (angstroms):

C1	-C2	:	1.406282	C1	-C6	:	1.389820
C1	-H111	:	1.085396	C2	-C3	:	1.408217
C2	-C7	:	1.464572	C3	-C4	:	1.387943
C3	-H108	:	1.087389	C4	-C5	:	1.403064
C4	-H109	:	1.087010	C5	-C6	:	1.401757
C5	-S17	:	1.781314	C6	-H110	:	1.084506
C7	-C8	:	1.348876	C7	-H107	:	1.089631
C8	-C9	:	1.461465	C8	-H106	:	1.088638
C9	-C10	:	1.408592	C9	-C14	:	1.407031
C10	-C11	:	1.387313	C10	-H103	:	1.087672
C11	-C12	:	1.402911	C11	-H102	:	1.084542
C12	-C13	:	1.402490	C12	-P15	:	1.843374
C13	-C14	:	1.391526	C13	-H105	:	1.086093
C14	-H104	:	1.086636	P15	-C16	:	1.848589
P15	-C19	:	1.846202	P15	-Co20	:	2.195987
C16	-H96	:	1.092729	C16	-H97	:	1.094902
C16	-H98	:	1.090994	S17	-C18	:	1.821474
C18	-H112	:	1.092184	C18	-H113	:	1.092851
C18	-H114	:	1.092645	C19	-H99	:	1.091778
C19	-H100	:	1.092049	C19	-H101	:	1.094821
Co20	-Se21	:	2.429300	Co20	-Se23	:	2.420922
Co20	-Se25	:	2.413802	Co20	-Se30	:	2.425260
Se21	-Co22	:	2.417383	Se21	-Co31	:	2.432388
Co22	-Se23	:	2.422111	Co22	-Se29	:	2.421243
Co22	-Se35	:	2.420731	Co22	-P46	:	2.185624
Se23	-Co24	:	2.417820	Co24	-Se25	:	2.422431
Co24	-Se27	:	2.426869	Co24	-Se29	:	2.421327
Co24	-P40	:	2.185246	Se25	-Co26	:	2.423503
Co26	-Se27	:	2.419058	Co26	-Se30	:	2.419884
Co26	-Se34	:	2.417915	Co26	-P36	:	2.185619
Se27	-Co28	:	2.423037	Co28	-Se29	:	2.427416
Co28	-Se34	:	2.417890	Co28	-Se35	:	2.412726
Co28	-P44	:	2.187189	Se30	-Co31	:	2.412442
Co31	-P32	:	2.185781	Co31	-Se34	:	2.414684
Co31	-Se35	:	2.415312	P32	-C33	:	1.845391
P32	-C52	:	1.844897	P32	-C53	:	1.845044
C33	-H84	:	1.095784	C33	-H85	:	1.092148
C33	-H86	:	1.092480	P36	-C37	:	1.845107
P36	-C38	:	1.845139	P36	-C39	:	1.843471
C37	-H90	:	1.095907	C37	-H91	:	1.092118
C37	-H92	:	1.092706	C38	-H87	:	1.095590
C38	-H88	:	1.092113	C38	-H89	:	1.092342
C39	-H93	:	1.095823	C39	-H94	:	1.092350
C39	-H95	:	1.092173	P40	-C41	:	1.844969
P40	-C42	:	1.846127	P40	-C43	:	1.844725
C41	-H69	:	1.095837	C41	-H70	:	1.092614
C41	-H71	:	1.092168	C42	-H72	:	1.095910
C42	-H73	:	1.092318	C42	-H74	:	1.092259
C43	-H75	:	1.095789	C43	-H76	:	1.091922
C43	-H77	:	1.092568	P44	-C45	:	1.835542
P44	-C50	:	1.848548	P44	-C51	:	1.846923

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 C45     -C115    :   1.401302      C45     -C119    :   1.403377
 P46     -C47     :   1.844192      P46     -C48     :   1.844976
 P46     -C49     :   1.845177      C47     -H63     :   1.096023
 C47     -H64     :   1.092138      C47     -H65     :   1.092649
 C48     -H60     :   1.095960      C48     -H61     :   1.092658
 C48     -H62     :   1.092248      C49     -H66     :   1.095739
 C49     -H67     :   1.092280      C49     -H68     :   1.092261
 C50     -H54     :   1.094228      C50     -H55     :   1.091771
 C50     -H56     :   1.092810      C51     -H57     :   1.094868
 C51     -H58     :   1.093105      C51     -H59     :   1.090682
 C52     -H81     :   1.095960      C52     -H82     :   1.092173
 C52     -H83     :   1.092538      C53     -H78     :   1.095962
 C53     -H79     :   1.092562      C53     -H80     :   1.091757
 C115    -C116    :   1.388919      C115    -H120    :   1.085966
 C116    -C117    :   1.406537      C116    -H121    :   1.088059
 C117    -C118    :   1.407800      C117    -C122    :   1.459779
 C118    -C119    :   1.388492      C118    -H123    :   1.085965
 C119    -H124    :   1.086225      C122    -C125    :   1.348296
 C122    -H126    :   1.087583      C125    -C127    :   1.461581
 C125    -H128    :   1.088872      C127    -C129    :   1.408583
 C127    -C133    :   1.407151      C129    -C130    :   1.385991
 C129    -H134    :   1.087681      C130    -C131    :   1.403935
 C130    -H135    :   1.087261      C131    -C132    :   1.400564
 C131    -S136    :   1.781530      C132    -C133    :   1.390476
 C132    -H137    :   1.084938      C133    -H138    :   1.084435
 S136    -C139    :   1.822200      C139    -H140    :   1.092103
 C139    -H141    :   1.092308      C139    -H142    :   1.092116

  bond angles:

 C6      -C1      -C2      : 121.696699  H111    -C1      -C2      :
120.190572
 H111    -C1      -C6      : 118.112585  C3      -C2      -C1      :
116.825392
 C7      -C2      -C1      : 123.934174  C7      -C2      -C3      :
119.235132
 C4      -C3      -C2      : 121.995701  H108    -C3      -C2      :
119.031719
 H108    -C3      -C4      : 118.971551  C5      -C4      -C3      :
120.362176
 H109    -C4      -C3      : 119.708475  H109    -C4      -C5      :
119.929248
 C6      -C5      -C4      : 118.468402  S17     -C5      -C4      :
116.931772
 S17     -C5      -C6      : 124.599772  C5      -C6      -C1      :
120.650391
 H110    -C6      -C1      : 118.731262  H110    -C6      -C5      :
120.618347
 C8      -C7      -C2      : 126.092518  H107    -C7      -C2      :
114.889715
 H107    -C7      -C8      : 119.002680  C9      -C8      -C7      :
128.522430
 H106    -C8      -C7      : 117.963906  H106    -C8      -C9      :
113.489976
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 C10     -C9      -C8      : 117.946352  C14     -C9      -C8      :
124.941685
 C14     -C9      -C10     : 117.095226  C11     -C10     -C9      :
121.775014
 H103    -C10     -C9      : 118.956841  H103    -C10     -C11     :
119.256001
 C12     -C11     -C10     : 120.855707  H102    -C11     -C10     :
118.765820
 H102    -C11     -C12     : 120.356571  C13     -C12     -C11     :
117.785863
 P15     -C12     -C11     : 118.958534  P15     -C12     -C13     :
123.234920
 C14     -C13     -C12     : 121.354097  H105    -C13     -C12     :
120.062742
 H105    -C13     -C14     : 118.576365  C13     -C14     -C9      :
121.126950
 H104    -C14     -C9      : 120.006641  H104    -C14     -C13     :
118.864567
 C16     -P15     -C12     : 101.931758  C19     -P15     -C12     :
102.267337
 C19     -P15     -C16     : 101.273861  Co20    -P15     -C12     :
117.526534
 Co20    -P15     -C16     : 115.920774  Co20    -P15     -C19     :
115.517486
 H96     -C16     -P15     : 108.314214  H97     -C16     -P15     :
110.955937
 H97     -C16     -H96     : 110.145215  H98     -C16     -P15     :
110.113652
 H98     -C16     -H96     : 107.356769  H98     -C16     -H97     :
109.874498
 C18     -S17     -C5      : 103.602514  H112    -C18     -S17     :
105.620221
 H113    -C18     -S17     : 111.641842  H113    -C18     -H112    :
108.777323
 H114    -C18     -S17     : 111.496835  H114    -C18     -H112    :
108.935677
 H114    -C18     -H113    : 110.203416  H99     -C19     -P15     :
108.473809
 H100    -C19     -P15     : 109.799785  H100    -C19     -H99     :
107.524223
 H101    -C19     -P15     : 110.989290  H101    -C19     -H99     :
110.159988
 H101    -C19     -H100    : 109.818588  Se21    -Co20    -P15     :
103.494711
 Se23    -Co20    -P15     : 101.225951  Se23    -Co20    -Se21    :
87.200400
 Se25    -Co20    -P15     :  96.369197  Se25    -Co20    -Se21    :
160.097036
 Se25    -Co20    -Se23    :  87.738520  Se30    -Co20    -P15     :
99.846578
 Se30    -Co20    -Se21    :  88.778485  Se30    -Co20    -Se23    :
158.908198
 Se30    -Co20    -Se25    :  89.053348  Co22    -Se21    -Co20    :
76.437469
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 Co31    -Se21    -Co20    :  75.093156  Co31    -Se21    -Co22    :
74.647969
 Se23    -Co22    -Se21    :  87.442652  Se29    -Co22    -Se21    :
161.180053
 Se29    -Co22    -Se23    :  87.782905  Se35    -Co22    -Se21    :
89.379548
 Se35    -Co22    -Se23    : 159.872533  Se35    -Co22    -Se29    :
88.867638
 P46     -Co22    -Se21    :  97.938039  P46     -Co22    -Se23    :
103.169792
 P46     -Co22    -Se29    : 100.874682  P46     -Co22    -Se35    :
96.952965
 Co22    -Se23    -Co20    :  76.505946  Co24    -Se23    -Co20    :
76.196762
 Co24    -Se23    -Co22    :  75.783864  Se25    -Co24    -Se23    :
87.612876
 Se27    -Co24    -Se23    : 160.350677  Se27    -Co24    -Se25    :
89.061566
 Se29    -Co24    -Se23    :  87.878772  Se29    -Co24    -Se25    :
161.294405
 Se29    -Co24    -Se27    :  89.107369  P40     -Co24    -Se23    :
101.844549
 P40     -Co24    -Se25    : 101.051987  P40     -Co24    -Se27    :
97.800108
 P40     -Co24    -Se29    :  97.640192  Co24    -Se25    -Co20    :
76.243161
 Co26    -Se25    -Co20    :  75.571036  Co26    -Se25    -Co24    :
74.874395
 Se27    -Co26    -Se25    :  89.218548  Se30    -Co26    -Se25    :
88.953025
 Se30    -Co26    -Se27    : 160.921918  Se34    -Co26    -Se25    :
160.020002
 Se34    -Co26    -Se27    :  87.653339  Se34    -Co26    -Se30    :
87.605199
 P36     -Co26    -Se25    :  96.596809  P36     -Co26    -Se27    :
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 P36     -Co26    -Se30    : 100.756977  P36     -Co26    -Se34    :
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 Co26    -Se27    -Co24    :  74.874335  Co28    -Se27    -Co24    :
74.959041
 Co28    -Se27    -Co26    :  76.033558  Se29    -Co28    -Se27    :
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 Se34    -Co28    -Se27    :  87.563477  Se34    -Co28    -Se29    :
159.780590
 Se35    -Co28    -Se27    : 160.768207  Se35    -Co28    -Se29    :
88.909625
 Se35    -Co28    -Se34    :  87.767024  P44     -Co28    -Se27    :
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 P44     -Co28    -Se29    :  98.313084  P44     -Co28    -Se34    :
101.906234
 P44     -Co28    -Se35    :  99.693567  Co24    -Se29    -Co22    :
75.735336
 Co28    -Se29    -Co22    :  75.100848  Co28    -Se29    -Co24    :
74.980037
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 Co26    -Se30    -Co20    :  75.427583  Co31    -Se30    -Co20    :
75.530017
 Co31    -Se30    -Co26    :  75.793951  Se30    -Co31    -Se21    :
89.003026
 P32     -Co31    -Se21    :  97.179844  P32     -Co31    -Se30    :
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 Se34    -Co31    -Se21    : 160.509774  Se34    -Co31    -Se30    :
87.848442
 Se34    -Co31    -P32     : 102.303363  Se35    -Co31    -Se21    :
89.154927
 Se35    -Co31    -Se30    : 161.527735  Se35    -Co31    -P32     :
100.637682
 Se35    -Co31    -Se34    :  87.781242  C33     -P32     -Co31    :
116.433902
 C52     -P32     -Co31    : 116.598710  C52     -P32     -C33     :
101.557925
 C53     -P32     -Co31    : 116.265122  C53     -P32     -C33     :
101.445359
 C53     -P32     -C52     : 102.091759  H84     -C33     -P32     :
110.543999
 H85     -C33     -P32     : 109.319104  H85     -C33     -H84     :
109.746921
 H86     -C33     -P32     : 109.147699  H86     -C33     -H84     :
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 H86     -C33     -H85     : 108.381840  Co28    -Se34    -Co26    :
76.150177
 Co31    -Se34    -Co26    :  75.789075  Co31    -Se34    -Co28    :
75.824356
 Co28    -Se35    -Co22    :  75.378082  Co31    -Se35    -Co22    :
74.896824
 Co31    -Se35    -Co28    :  75.908221  C37     -P36     -Co26    :
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 C38     -P36     -Co26    : 115.976375  C38     -P36     -C37     :
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 C39     -P36     -Co26    : 116.399356  C39     -P36     -C37     :
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 C39     -P36     -C38     : 101.760469  H90     -C37     -P36     :
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 H91     -C37     -P36     : 109.528183  H91     -C37     -H90     :
109.735554
 H92     -C37     -P36     : 109.127987  H92     -C37     -H90     :
109.632314
 H92     -C37     -H91     : 107.927460  H87     -C38     -P36     :
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 H88     -C38     -P36     : 109.411939  H88     -C38     -H87     :
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 H89     -C38     -P36     : 109.089373  H89     -C38     -H87     :
109.610109
 H89     -C38     -H88     : 108.368090  H93     -C39     -P36     :
110.682170
 H94     -C39     -P36     : 109.349549  H94     -C39     -H93     :
109.695853
 H95     -C39     -P36     : 109.474688  H95     -C39     -H93     :
109.743478
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 H95     -C39     -H94     : 107.843795  C41     -P40     -Co24    :
116.772970
 C42     -P40     -Co24    : 115.717423  C42     -P40     -C41     :
101.574504
 C43     -P40     -Co24    : 116.853939  C43     -P40     -C41     :
101.967878
 C43     -P40     -C42     : 101.487054  H69     -C41     -P40     :
110.723888
 H70     -C41     -P40     : 109.146395  H70     -C41     -H69     :
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 H71     -C41     -P40     : 109.592745  H71     -C41     -H69     :
109.781736
 H71     -C41     -H70     : 107.847851  H72     -C42     -P40     :
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 H73     -C42     -P40     : 109.164274  H73     -C42     -H72     :
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 H74     -C42     -P40     : 109.132787  H74     -C42     -H72     :
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 H74     -C42     -H73     : 108.305985  H75     -C43     -P40     :
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 H76     -C43     -P40     : 109.595366  H76     -C43     -H75     :
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 H77     -C43     -P40     : 109.080010  H77     -C43     -H75     :
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 H77     -C43     -H76     : 107.994593  C45     -P44     -Co28    :
118.208553
 C50     -P44     -Co28    : 115.515702  C50     -P44     -C45     :
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 C51     -P44     -Co28    : 115.004146  C51     -P44     -C45     :
102.700816
 C51     -P44     -C50     : 100.779068  C115    -C45     -P44     :
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 C119    -C45     -P44     : 121.985774  C119    -C45     -C115    :
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 C47     -P46     -Co22    : 116.556715  C48     -P46     -Co22    :
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 C48     -P46     -C47     : 102.313442  C49     -P46     -Co22    :
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 C49     -P46     -C47     : 101.727263  C49     -P46     -C48     :
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 H63     -C47     -P46     : 110.700417  H64     -C47     -P46     :
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 H61     -C48     -H60     : 109.637316  H62     -C48     -P46     :
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 H62     -C48     -H60     : 109.733735  H62     -C48     -H61     :
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 H66     -C49     -P46     : 110.644577  H67     -C49     -P46     :
109.095478
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 H68     -C49     -H66     : 109.789573  H68     -C49     -H67     :
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 H55     -C50     -H54     : 109.881633  H56     -C50     -P44     :
107.783008
 H56     -C50     -H54     : 110.333460  H56     -C50     -H55     :
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