Supporting Information

The approach to 4d/4f-Polyphosphides

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Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x
Experimental

General Considerations
All manipulations of air-sensitive materials were performed with the rigorous exclusion of oxygen and moisture in flame-dried Schlenk-type glassware either on a dual manifold Schlenk line, interfaced to a high vacuum (10⁻³ torr) line, or in an argon-filled MBraun glove box. Elemental analyses were carried out with an Elementar vario Micro Cube. Hydrocarbon solvents were predried by using an MBraun solvent purification system (SPS-800) and degassed, dried and stored in vacuo over LiAlH₄. Tetrahydrofuran was distilled under nitrogen from potassium benzophenone ketyl before storage over LiAlH₄. IR spectra were obtained on a Bruker Tensor 37 FTIR spectrometer equipped with a room temperature DLaTGS detector and a diamond ATR (attenuated total reflection) unit; for the mid infrared region a KBr beamsplitter was used. [Cp*₂Ln(thf)₂] (Ln = Sm, Yb),¹⁻³ [{CpMo(CO)₂}₂(µ,η²⁻²⁻₂-P₂)]₄ and [Cp*Mo(CO)₂(η³⁻₃⁻₃)]⁵ were prepared according to literature procedures.

Near infrared absorbance (NIR) measurements of 1a and 4
NIR measurements of 1a and 4 were performed with the help of an ATR diamond at room temperature using the FTIR spectrometer Bruker Tensor 37 by means of an NIR lamp, a CaF₂ beamsplitter and a room temperature InGaAs detector (Figure S3 and S11).

Magnetic Measurements
The magnetic measurements were carried out with the use of a Quantum Design SQUID magnetometer MPMS-XL in the temperature range 1.8 - 300 K and with dc applied fields ranging from 7 to -5 T. Measurements were performed on the polycrystalline samples with extreme caution. The sample bag was prepared in glove box, sealed under argon and transferred into the magnetometer immediately. The magnetic data were corrected for the sample holder.

General procedure for ampoule reactions
For the synthesis and recrystallization, two-section and three-section ampoules were used (see . The starting compounds were loaded into one section of the ampoule in an argon-filled glove box. The section with the starting materials was cooled by immersion in a liquid nitrogen bath, and the required solvent (typically 10 mL of solvent) was condensed in vacuo onto the starting materials. The ampoule was then flame-sealed. The reaction mixture was slowly warmed up to room temperature and then heated to 60 °C until the color had definitely changed from purple to red-brown. If a precipitate formed, the product was separated by decantation of the solution to another section of the ampoule. A concentrated solution was obtained by slow evaporation of
the solvent to the empty section of the ampoule. Crystals were obtained at room temperature and isolated by decantation of the solution to the other section of ampoule followed by drying by means of cooling the section with the mother liquor. The section with crystals was flame-sealed and opened in a glovebox.

Figure S1: (a) Two section and (b) three section ampoule.

\[(\text{Cp}^*_{2}\text{Sm})_2\text{P}_2(\text{CpMo(CO)}_2)_4\] (1a)

In a three-section-ampoule, toluene (15 mL) was condensed at -78 °C onto a mixture of [Cp*2Sm(thf)_2] (80 mg, 0.14 mmol) and \([\text{CpMo(CO)}_2]_2(\mu,\eta^{2,2}\text{-P}_2)] (70 mg, 0.141 mmol). The resulting dark red reaction solution was heated for one week at 60° C. After two weeks at room temperature red crystals of \([(\text{Cp}^*_2\text{Sm})_2\text{P}_2(\text{CpMo(CO)}_2)_4]\) were obtained. The supernatant solution was decanted and the section with \([(\text{Cp}^*_2\text{Sm})_2\text{P}_2(\text{CpMo(CO)}_2)_4]\) was flame-sealed. Yield: 10 mg, 7 % (single crystals).

IR (ATR, \(\tilde{\nu}/\text{cm}^{-1}\)): 2906 (vw), 2855 (w), 1945 (s), 1905 (vs), 1871 (vs), 1683 (vs), 1636 (s), 1423 (w), 1382 (w), 1058 (w), 1007 (w), 811 (vs), 789 (vs), 727 (vw), 693 (vw), 661 (vw), 557 (s), 531 (m).NIR (ATR, \(\tilde{\nu}/\text{cm}^{-1}\)): 9319 (m), 9217 (vw), 9151 (m), 9058 (w), 8968 (w), 8217 (s), 8158 (vw), 8048 (vs), 7960 (w), 7791 (w), 7338 (m), 7236 (vw), 7171 (vw), 6388 (w), 6126 (vw). Anal. Calc. for C_{68}H_{80}Mo_{4}O_{8}P_{2}Sm_{2} (1771.89 g·mol⁻¹) (1 – 1 Tol): C, 46.09; H, 4.55. Found: C, 46.01; H, 4.32.

\([(\text{Cp}^*_2\text{Sm})_2\text{P}_4(\text{CpMo(CO)}_2)_2]\) (2) and \([(\text{Cp}^*_2\text{Sm})_3\text{P}_5(\text{CpMo(CO)}_2)_3]\) (3)

From the remaining reaction mixture from 1a, small amounts of two different kinds of orange crystals were obtained by slow evaporation. Due to the similar solubility and the low yields of the two products, no further analytical data could be collected.
[(Cp*₂Yb)₂P₂(CpMo(CO)₂)₄] (1b)

In a two-section ampoule, toluene (15 mL) was condensed at -78 °C onto a mixture of [Cp*₂Yb(thf)₂] (82 mg, 0.14 mmol) and [{CpMo(CO)₂}₂(μ,η²⁻²-P₂)] (70 mg, 0.141 mmol). The resulting dark red reaction solution was heated for one week at 60° C. After two weeks at room temperature, crystals of [(Cp*₂Yb)₂(CpMo(CO)₂)₄P₂] were obtained. Yield: 8 mg, 6 % (single crystals).

IR (ATR, ν/cm⁻¹): 2900 (w), 2856 (w), 1906 (vs), 1874 (vs), 1687 (vs), 1638 (s), 1486 (vw), 1432 (m), 1382 (w), 1107 (vw), 1059 (w), 1007 (m), 790 (s), 727 (w), 696 (vw), 585 (m), 553 (s), 504 (m). Anal. Calc. for C₆₈H₈₆O₅₆P₂Yb₂ (1817.10 g·mol⁻¹): C, 44.49; H, 4.44. Found: C, 44.76; H, 4.27.

[(Cp*₂Sm)₂P₆(Cp*Mo(CO)₂)₄] (4)

Toluene (15 mL) was condensed at -78 °C onto a mixture of [Cp*₂Sm(thf)₂] (178 mg, 0.316 mmol) and [Cp*Mo(CO)₂(η²⁻³-P₃)] (120 mg, 0.316 mmol). The resulting reaction mixture was heated for one week at 60 °C. After two weeks at room temperature, crystals of [(Cp*₂Sm)₂P₆(Cp*Mo(CO)₂)₄] were obtained. Yield: 20 mg, 14 % (single crystals).

IR (ATR, ν/cm⁻¹): 2958 (m), 2901 (s), 2853 (s), 2722 (vw), 1983 (m), 1917 (vs), 1701 (vs), 1646 (m), 1477 (w), 1442 (m), 1377 (m), 1150 (vw), 1104 (w), 1067 (w), 1026 (m), 799 (vw), 728 (m), 693 (w), 607 (vw), 555 (m), 515 (w). NIR (ATR, ν/cm⁻¹): 9489 (vs), 9224 (vw), 9109 (vs), 8719 (w), 8107 (s), 7967 (vs), 7781 (w), 7338 (w), 7236 (w), 7152 (w), 6702 (m), 6566 (w), 6395 (w), 6325 (w). Anal. Calc. for C₇₁H₉₈O₂₄P₆Sm₂ (1694.04 g·mol⁻¹) (4 – 1Tol): C, 50.34; H, 5.83. Found: C, 50.46; H, 6.02.

[(Cp*₂Yb)₂P₆(Cp*Mo(CO)₂)₄] (5)

Toluene (15 mL) was condensed at -78 °C onto a mixture of [Cp*₂Yb(thf)₂] (157 mg, 0.273 mmol) and [Cp*Mo(CO)₂(η³⁻³-P₃)] (102 mg, 0.273 mmol). The resulting reaction mixture was heated for one week at 60 °C. After two weeks at room temperature, black needles of [(Cp*₂Yb)₂P₆(Cp*Mo(CO)₂)₄] were obtained. Yield: 14 mg, 18 % (single crystals). IR (ATR, ν/cm⁻¹): 3023 (vw), 2899 (s), 2854 (s), 2721 (vw), 1985 (w), 1916 (vs), 1737 (w), 1696 (vs), 1669 (s), 1493 (w), 1477 (w), 1445 (m), 1376 (m), 1310 (vw), 1240 (w), 1155 (vw), 1066 (m), 1025 (m), 798 (w), 728 (m), 693 (w), 609 (w), 555 (m). Anal. Calc. for C₆₇H₉₄O₂₄P₆Yb₂ (1687.36 g·mol⁻¹) (5 – 0.5 Tol): C, 47.69; H, 5.62. Found: C, 48.14; H, 5.03.
X-ray Crystallographic Studies of 1-5

A suitable crystal was covered in mineral oil (Aldrich) and mounted on a glass fiber. The crystal was transferred directly to a cold stream of a STOE IPDS 2, STOE StadiVari or Xcalibur diffractometer.

All structures were solved using SHELXS-2013. The remaining non-hydrogen atoms were located from successive difference Fourier map calculations. The refinements were carried out by using full-matrix least-squares techniques on \( F \), minimizing the function \( (F_o-F_c)^2 \), where the weight is defined as \( 4F_o^2/2(F_o)^2 \) and \( F_o \) and \( F_c \) are the observed and calculated structure factor amplitudes using the program SHELXL-2013. Hydrogen atom positions were calculated. The locations of the largest peaks in the final difference Fourier map calculation as well as the magnitude of the residual electron densities in each case were of no chemical significance. Positional parameters, hydrogen atom parameters, thermal parameters, bond distances and angles have been deposited as supporting information.

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication no. CCDC 1402049-1402054. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

Crystal data for 1a: \( \text{C}_{68}\text{H}_{80}\text{Mo}_4\text{O}_8\text{P}_2\text{Sm}_2\text{C}_7\text{H}_8, \, M = 1863.85, \, a = 9.5023(3) \, \text{Å}, \, b = 12.6103(4) \, \text{Å}, \, c = 15.1418(5) \, \text{Å}, \, \alpha = 97.784(3)^\circ, \, \beta = 90.790(3)^\circ, \, \gamma = 100.069(3)^\circ, \, V = 1768.68(10) \, \text{Å}^3, \, T = 100 \, \text{K}, \, Z = 1, \, 17149 \, \text{reflections measured, 6969 independent reflections} \, (R_{int} = 0.0684). \) The final \( R_f \) values were 0.0516 \((I > 2\sigma(I))\). The final \( wR(F^2) \) values were 0.1266 \((I > 2\sigma(I))\). The final \( R_f \) values were 0.0715 (all data). The final \( wR(F^2) \) values were 0.1389 (all data). The goodness of fit on \( F^2 \) was 0.997.

Crystal data for 1b: \( \text{C}_{68}\text{H}_{80}\text{Mo}_4\text{O}_8\text{P}_2\text{Yb}_2, \, M = 1817.10, \, a = 9.4563(7) \, \text{Å}, \, b = 12.5189(13) \, \text{Å}, \, c = 14.9787(13) \, \text{Å}, \, \alpha = 84.903(8)^\circ, \, \beta = 71.669(7)^\circ, \, \gamma = 76.285(7)^\circ, \, V = 1635.0(3) \, \text{Å}^3, \, T = 150 \, \text{K}, \, Z = 1, \, 14805 \, \text{reflections measured, 5918 independent reflections} \, (R_{int} = 0.0698). \) The final \( R_f \) values were 0.0392 \((I > 2\sigma(I))\). The final \( wR(F^2) \) values were 0.0708 \((I > 2\sigma(I))\). The final \( R_f \) values were 0.0654 (all data). The final \( wR(F^2) \) values were 0.0772 (all data). The goodness of fit on \( F^2 \) was 0.945.

Crystal data for 2: \( \text{C}_{54}\text{H}_{70}\text{Mo}_2\text{O}_4\text{P}_4\text{Sm}_2\text{2(C}_7\text{H}_8), \, M = 1583.82, \, a = 9.6185(7) \, \text{Å}, \, b = 10.2667(7) \, \text{Å}, \, c = 17.5096(13) \, \text{Å}, \, \alpha = 83.519(6)^\circ, \, \beta = 77.307(6)^\circ, \, \gamma = 78.461(6)^\circ, \, V = 1648.44(21) \, \text{Å}^3, \, T = 100 \, \text{K}, \, Z = 1, \, 12256 \, \text{reflections measured, 5964 independent reflections} \, (R_{int} = 0.1155). \) The final \( R_f \) values were 0.0708 \((I > 2\sigma(I))\). The final \( wR(F^2) \) values were 0.1908 \((I > 2\sigma(I))\).
$2\sigma(I)$. The final $R_I$ values were 0.0860 (all data). The final $wR(F^2)$ values were 0.2034 (all data). The goodness of fit on $F^2$ was 1.062.

Crystal data for 3: $\text{C}_81\text{H}_{105}\text{Mo}_3\text{O}_6\text{P}_5\text{Sm}_3$, $M = 2068.36$, $a = 10.130(2) \text{ Å}$, $b = 25.686(5) \text{ Å}$, $c = 15.724(3) \text{ Å}$, $\alpha = 90^\circ$, $\beta = 96.36(3)^\circ$, $\gamma = 90^\circ$, $V = 4066.3(14) \text{ Å}^3$, $T = 100 \text{ K}$, space group $P121/m1$, $Z = 2$, 33852 reflections measured, 7394 independent reflections ($R_{int} = 0.2911$). The final $R_I$ values were 0.1092 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.2500 ($I > 2\sigma(I)$). The final $R_I$ values were 0.1889 (all data). The final $wR(F^2)$ values were 0.2946 (all data). The goodness of fit on $F^2$ was 0.980.

Crystal data for 4: $\text{C}_{64}\text{H}_{90}\text{Mo}_2\text{O}_4\text{P}_6\text{Sm}_2\cdot 2(\text{C}_7\text{H}_8)$, $M = 1786.02$, $a = 11.1671(8) \text{ Å}$, $b = 12.7931(10) \text{ Å}$, $c = 14.7276(9) \text{ Å}$, $\alpha = 98.952(6)^\circ$, $\beta = 110.227(6)^\circ$, $\gamma = 95.319(6)^\circ$, $V = 1925.7(2) \text{ Å}^3$, $T = 123 \text{ K}$, space group $P-1$, $Z = 1$, 15246 reflections measured, 6698 independent reflections ($R_{int} = 0.0368$). The final $R_I$ values were 0.0343 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0799 ($I > 2\sigma(I)$). The final $R_I$ values were 0.0368 (all data). The final $wR(F^2)$ values were 0.0815 (all data). The goodness of fit on $F^2$ was 0.980. 

Crystal data for 5: $\text{C}_{64}\text{H}_{90}\text{Mo}_2\text{O}_4\text{P}_6\text{Yb}_2\cdot 2(\text{C}_7\text{H}_8)$, $M = 1831.40$, $a = 11.1924(3) \text{ Å}$, $b = 12.6285(3) \text{ Å}$, $c = 14.6371(4) \text{ Å}$, $\alpha = 99.581(2)^\circ$, $\beta = 110.455(2)^\circ$, $\gamma = 94.847(2)^\circ$, $V = 1888.44(9) \text{ Å}^3$, $T = 100 \text{ K}$, space group $P-1$, $Z = 1$, 17122 reflections measured, 7340 independent reflections ($R_{int} = 0.0260$). The final $R_I$ values were 0.0410 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1014 ($I > 2\sigma(I)$). The final $R_I$ values were 0.0447 (all data). The final $wR(F^2)$ values were 0.1033 (all data). The goodness of fit on $F^2$ was 1.084.
Figure S2. IR-spectrum of 1a.

Figure S3. NIR-spectrum of 1a.
Figure S4. IR-spectrum of 1b.
**Figure S5.** Solid-state structure of 3 showing the full disordered of the central P₅-core. Hydrogen atoms are omitted for clarity.

**Figure S6.** Solid-state structure of 3 showing each part of the disordered structure separated.
**Figure S7.** Solid-state structure of 4 showing the full disordered of the central P₆-core. Hydrogen atoms are omitted for clarity.

**Figure S8.** Solid-state structure of 4 showing the four-fold disordering of the central P₆-core only.
Figure S9. Temperature-dependent SQUID magnetization data for 4. $\chi M$ versus $T$ plot at 1000 Oe and $M$ versus $T$ plot.
Figure S10. IR-spectrum of 4.

Figure S11. NIR-spectrum of 4.
Figure S12. IR-spectrum of 5.
**Supplemental contribution/quantum chemical calculations**

*Table S1*: Results of the quantum chemical calculations (distances given in Å; shared electron numbers SEN and partial charges Q determined by Ahlrichs-Heinzmann population analysis, each 10 MAOs chosen for Sm and Mo) on 1a, 2, 3, and [\{CpMo(CO)\}_2(\mu,\eta^{2-2}:2\_2-P_2)]

|            | 1a       | 2          | 3           | 4          |
|------------|----------|------------|-------------|------------|
| r(P-P)     | 2.078    | 2.181      | 2.205       | 2.121      |
|            | (P1-P2, P1′-P2’), (P1-P2’, P1′-P2) | (P1-P5, P4-P5), (P3-P4), (P1-P2), (P2-P3) | (Mo2′-P5), (Mo2-P4), (Mo1-P1), (Mo2-P3), (Mo1-P2) |
| r(Mo-P)    | 2.406    | 2.568      | 2.394       | 2.505      |
|            | (Mo’-P1’, Mo-P1) | (Mo2′-P5) | (Mo2-P4), (Mo1-P1), (Mo2-P3), (Mo1-P2) |
| r(Mo-Mo)   | 3.247    | 3.087      |             |            |
|            |          |            |             |            |
| SEN(P-P)   | 1.38     | 1.24       | 1.12        | 1.41       |
|            | (P1-P2, P1′-P2’), (P1-P2’, P1′-P2) | (P1-P5, P4-P5), (P3-P4), (P1-P2), (P2-P3) |
| SEN(Mo-P)  | 0.77     | 0.59       | 0.66        | 0.55       |
|            |          |            | (Mo2′-P5), (Mo2-P4), (Mo1-P1), (Mo2-P3), (Mo1-P2) |
| SEN(Mo-Mo) | 0.23     |            |             | 0.30       |
| SEN(Sm-P)  |          |            |             |            |
| Q(Sm)      | 1.04     | 0.38       |             |            |
|            | Sm1: 0.35 | Sm1′: 1.21 |             |            |
| Q(Mo)      | -0.52    | -0.52      |            | -0.54      |
|            | Mo1: -0.45 | Mo2: -0.45 |            |            |
| Q(P)       | 0.02     | 0.03       |             | 0.07       |
|            | P1: -0.20 | P2: -0.08  |            |            |
|            | P3: 0.00  | P4: -0.01  |            |            |
|            | P5: -0.08 |            |            |            |
Table S2: Results of the quantum chemical calculations (distances given in Å; shared electron numbers SEN and partial charges Q determined by Ahlrichs-Heinzmann population analysis) on the model compounds Na₄P₂⁺, Na₂P₄, NaP₅ and Na₃P₅²⁺ as well as Tₐ and D₂h-P₄.

|          | Na₄P₂⁺ | Na₂P₄ | NaP₅     | Na₃P₅²⁺     | P₄     | P₄     |
|----------|--------|--------|-----------|--------------|--------|--------|
| symmetry | D₂h    | D₄h    | C₅v       | Cₛ           | Tₐ     | D₂h    |
| r(P-P)   | 2.063  | 2.168  | 2.147     | 2.112/2.122/213.0 | 2.233  | 207.9/235.2 |
| SEN(P-P) | 1.74   | 1.44   | 1.38      | 1.43/1.38/1.33 | 1.08   | 1.66/0.96 |
| Q(Na)    | 0.56   | 0.40   | 0.54      | 0.69         | 0.00   | 0.00   |
| Q(P)     | -0.12  | -0.20  | -0.11     | -0.01        | 0.00   | 0.00   |
Figure S13: Comparison of the MO diagrams of $\text{Na}_4\text{P}_2^{2+}$ and $[(\text{Cp}_2^*\text{Ln})_2\text{P}_2(\text{CpMo(CO)}_2)_4]$. Only the MOs with strong phosphorus contribution are shown.
Cartesian Coordinates of the calculated Molecules (given in a.u.)

\[
[(\text{Cp}_2^*\text{Ln})_2\text{P}_2\text{(CpMo(CO)}_2)_4] (1a)
\]

| X | Y | Z |
|---|---|---|
| 1.90296250200252 | -13.82810402990115 | 8.09534720152958 | h |
| 0.08122360005252 | -14.84040850928407 | 10.74781306916709 | h |
| 1.37981219598989 | -13.32230364685989 | 10.06893260714207 | c |
| 0.14023700628127 | -10.76210982108238 | 10.25462714082543 | c |
| 3.1204111688955 | -13.44572239584814 | 11.22950563951258 | h |
| 2.10081351152728 | -6.38499874179512 | 8.10304734795473 | sm |
| 0.36366432516577 | -9.00335622785759 | 12.3214915344817 | c |
| -1.7962348133009 | -9.84804709039902 | 8.58549018910282 | c |
| 0.74308860372980 | -6.52505761835600 | 3.74200396442685 | o |
| 0.55006996143110 | -10.76210982108238 | 10.25462714082543 | c |
| -2.76637565189906 | -7.53050742569598 | 9.60853311748393 | c |
| -1.42366475650434 | -9.99774888538406 | 11.9095396437644 | c |
| 6.59214457568642 | -4.82088920278127 | 6.0503453375946 | c |
| 6.84055093745446 | -7.51591578600646 | 6.30229819199671 | c |
| 7.00357581750721 | -8.09883668028852 | 8.95233193438237 | c |
| 6.82253254791578 | -5.76266175750081 | 10.33650701072655 | c |
| 6.58097647407015 | -3.74159490644463 | 8.5383257999748 | c |
| 1.83565304463779 | -9.4245544331244 | 14.72342686216367 | c |
| -2.81897132871851 | -11.23170169726158 | 6.3146826412209 | c |
| -0.2573280101706 | -6.08509094503992 | 1.71864829632883 | c |
| -0.29226672059125 | -2.51953974476834 | 6.75040026413424 | c |
| -4.96436167458927 | -6.05287487093342 | 8.56357474596062 | c |
| -1.95925550299904 | -4.84723930856814 | 13.70685594311421 | c |
| 6.53843689964543 | -3.36492024515305 | 3.60630507641387 | c |
| 7.12839272145268 | -9.37755587432994 | 4.16086286352399 | c |
| 7.73553347801920 | -10.629391980644 | 10.0357038178459 | c |
| 7.25195465521446 | -5.41403176764349 | 13.1335852581672 | c |
| 6.58115131985332 | -0.96191815085404 | 9.15814758903328 | c |
| 3.55942517508755 | -10.58232404058777 | 14.41696181079272 | h |
| 0.66564457039766 | -10.4496706428769 | 16.15027788527431 | c |
| 2.44074033724475 | -7.62597064815908 | 15.62334787555756 | h |
| -3.63462123703807 | -9.91962524821820 | 4.89291852001703 | h |
| -4.34919120763490 | -12.57477720958195 | 6.86671597940872 | h |
| -1.34427200254111 | -12.36323561746168 | 5.33458984730631 | h |
| -1.91568940289937 | -5.60200474798470 | -1.42106077117737 | mo |
| -1.86859755728729 | 2.54827595541933 | 5.1618297209614 | mo |
| -5.08695350119064 | -4.14163997599047 | 9.41961247870102 | h |
| -6.79600878437607 | -7.02234635720474 | 8.95559475085843 | h |
| -4.84043706181788 | -5.80220804368047 | 6.4787080457220 | h |
| -0.27114389931516 | -4.32849299549892 | 14.84531943591733 | h |
| -3.48030741705067 | -5.34959258230432 | 15.07890028353203 | h |
| -2.58659666915900 | -3.10994889237606 | 12.70622496804775 | h |
| 5.87668763886548 | -4.55495296959470 | 2.01208459085636 | h |
| 8.45888575115996 | -2.65290928393182 | 3.0977551751398 | c |
| 5.25629218508848 | -1.70101338418695 | 3.69318293384980 | h |
| 6.55298694373891 | -11.32028788671585 | 4.71748877880993 | h |
| 9.13242693655519 | -9.5038404912191 | 3.51487395309791 | h |
| 5.98101926733474 | -8.85021014010406 | 2.4815435279007 | h |
| 7.07321359758569 | -10.87852270491502 | 12.01370648789211 | h |
| x          | y          | z          |
|------------|------------|------------|
| 6.177937    | 38316183   | -5.960337   |
| 0.226776    | 14573054   | -1.405143   |
| 5.659157    | 12963444   | -2.246826   |
| 5.166154    | 3259538    | -7.292658   |
| 5.531935    | 40433425   | -9.625494   |
| -0.742579   | 97887000   | 6.524069    |
| -2.031182   | 70230548   | 3.269253    |
| 5.233600    | 02250497   | 5.920619    |
| 4.542406    | 98753134   | 5.164946    |
| 5.026386    | 66691597   | 1.030050    |
| 6.459061    | 14705086   | 5.932772    |
| 6.893418    | 86067227   | 2.270700    |
| -1.009890   | 42455774   | 6.385453    |
| 2.766141    | 44127141   | 7.530983    |
| 1.423209    | 03211511   | 6.998511    |
| -0.364158   | 50451087   | 9.004759    |
| -0.140567   | 77863877   | 10.762660   |
| 1.796071    | 93973035   | 9.848416    |
| -6.591171   | 45668873   | 4.820331    |
| -6.840944   | 41819079   | 7.515319    |
| -7.004088   | 85915948   | 8.098527    |
| -6.822555   | 1239731    | 5.762548    |
| -6.580516   | 66684793   | 3.741329    |
| 4.964237    | 76096487   | 6.053205    |
| 1.985725    | 932965891  | 4.848191    |
| -1.836324   | 33239785   | 9.425620    |
| -1.380323   | 0596018    | 13.322954   |
| 2.818951    | 81925620   | 11.231779   |
| -6.537811   | 76308071   | 3.364075    |
| -7.129028   | 8179112    | 9.376633    |
| -7.736297   | 76005705   | 10.629158   |
| -7.251838   | 87663626   | 5.414180    |
| -6.580057   | 7094202   | 0.961744    |
| 5.086844    | 97075626   | 4.142007    |
| 6.795932    | 26234667   | 7.022805    |
| 4.840220   | 20214490   | 5.802100    |
| 0.270611    | 64764488   | 4.329693    |
| 3.479943    | 66237748   | 5.350598    |
| 2.585873    | 67304038   | 3.110691    |
| -3.560017   | 76453966   | 10.583464   |
| -0.666381   | 19309839   | 10.450761   |
| -2.441582   | 29073152   | 7.627111    |
| -1.903575   | 47890872   | 13.828063   |
| -0.081878   | 863753905  | 14.841139   |
| -3.120861   | 91084599   | 13.446178   |
| 3.634022    | 95700814   | 9.919401    |
| 4.349401    | 3982467   | 12.574759   |
| 1.344956    | 2017933   | 12.363401   |
| -5.876139   | 94499074   | 4.554021    |
| -8.458003   | 3091292    | 2.651625    |
| -5.255320   | 44133424   | 1.700462    |
| -6.554013   | 24132169   | 11.319555   |
\[
\begin{array}{ccc}
-9.1330251918207 & 9.5024586215460 & -3.51422366590463 \\
-5.98139669633593 & 8.84930784219754 & -2.48120739149490 \\
-7.07401260858620 & 10.87361704232697 & -12.01307262599672 \\
-9.83489137131778 & 10.84642139808900 & -10.07147179913171 \\
-6.02732439039822 & 3.9162634489148 & -13.95905188231414 \\
-9.24315266968684 & 4.83749700284766 & -13.52623217032422 \\
-8.54787551148369 & 21.14401058843515 & -9.2955843037465 \\
-5.64211267290813 & 0.5476525760901 & -10.99200879312267 \\

\end{array}
\]

\[[(\text{Cp}_2\text{Sm})_2\text{P}_4(\text{CpMo(CO)}_2)_2]\] (2)

\begin{array}{ccc}
8.72787639556319 & 18.22119582848562 & 0.69659456858620 \\
9.81668776807678 & 19.77199636408579 & 1.54388457822821 \\
8.90823216450519 & 23.88351186865954 & 2.13875419911116 \\
9.87633921287200 & 20.41903412356979 & 4.18100157361666 \\
11.46419413739650 & 21.45831249219117 & 0.22342883433466 \\
8.73346967779394 & 28.56559555552543 & 0.91914096257979 \\
6.64047391697562 & 26.31768012858825 & -1.83028146273638 \\
12.5414891386481 & 23.16580299137826 & 2.02865863471603 \\
11.57062558791290 & 22.5249859228827 & 4.47390202461685 \\
4.64066896627686 & 22.40228518809662 & 1.61978178874903 \\
6.5298710989899 & 25.5331961493463 & 4.94649212754636 \\
8.84080772707888 & 19.42342972102186 & 5.70601574068083 \\
11.84619226578944 & 21.43465045712348 & -1.81553096280882 \\
5.00216077994619 & 30.71008440202762 & 1.83069428221617 \\
2.9094236642540 & 28.46333591501570 & -0.9189855518862 \\
13.90030661154894 & 24.6777684771742 & 1.61801582121453 \\
12.08623310770926 & 23.43561499488256 & 6.26588965250488 \\
2.69407272318160 & 21.36572801637471 & 1.39370616314467 \\
5.68430000544999 & 26.55537032577432 & 6.82027993667209 \\
3.63469336194828 & 33.14379610582645 & -2.1386268960521 \\
3.71053307478081 & 30.68204083518789 & 7.47783473408090 \\
1.82610224029104 & 37.25546204118324 & -1.54324981367439 \\
1.76565715114638 & 36.60922022652844 & -4.18046879785862 \\
-0.89383921158888 & 33.86174474509598 & -2.02810451649195 \\
0.07132021464554 & 34.50339813905457 & -4.47332110014742 \\
7.00253943473107 & 34.62465786036091 & -1.62029813733573 \\
0.17933517170039 & 35.56859117666363 & -0.2225908458733 \\
5.11283491527884 & 31.4936705589496 & -4.94765151874159 \\
-1.37021403315424 & 31.6530137391701 & 8.4180539829015 \\
-0.50290529496025 & 30.32203697255070 & 10.62681897132904 \\
-0.460478425891138 & 27.51197920919536 & 7.24656862710402 \\
-1.3675640399119 & 29.90613941251886 & 6.33664146549575 \\
0.09967110742449 & 27.77718347827180 & 9.88794098987887 \\
8.14240458450512 & 33.5827268670669 & 7.39591456433979 \\
6.89758279764969 & 32.0808222941581 & 11.3367367131459 \\
8.5643358878847 & 31.63707419674607 & 9.23622089721912 \\
6.19048413358778 & 35.226046791827 & 8.34403426882082 \\
5.45914462900263 & 34.33150406138315 & 10.80189157148066 \\
2.91500910110592 & 38.80663464488327 & -0.69545446150131 \\
\end{array}
\]
| x      | y      | z      | label |
|--------|--------|--------|-------|
| 2.75845896847627 | 37.6049706420030 | -5.70501542104746 | h   |
| -2.25751395459107 | 32.3501915163637 | -1.6170442708292 | h   |
| -0.44373258404788 | 33.59265307874583 | -6.2649237798292 | c   |
| 8.95006264001388 | 35.66079370381851 | -1.3943644871729 | h   |
| -0.20296041430407 | 35.9293207708095 | 1.81664044781729 | o   |
| 1.95719725725040 | 30.47216912638217 | -6.8200678828531 | o   |
| -2.46590259546941 | 34.2874436363222 | 8.3725346383923 | c   |
| -0.73196661440610 | 31.2813695447926 | 13.3205100943073 | c   |
| -0.39294732734577 | 32.1027761649005 | 5.7360856408058 | c   |
| -2.50890102072492 | 30.326532302446 | 3.7633445610545 | c   |
| 0.90166795088517 | 25.68157745109736 | 11.6473839870256 | c   |
| 9.76414965025097 | 34.0883429121748 | 5.1119215924331 | c   |
| 6.93443408839721 | 30.63643162173187 | 13.7964408363478 | c   |
| -2.46590259546941 | 34.2874436363222 | 8.3725346383923 | c   |
| -0.73196661440610 | 31.2813695447926 | 13.3205100943073 | c   |
| -0.39294732734577 | 32.1027761649005 | 5.7360856408058 | c   |
| -2.50890102072492 | 30.326532302446 | 3.7633445610545 | c   |
| 0.90166795088517 | 25.68157745109736 | 11.6473839870256 | c   |
| 9.76414965025097 | 34.0883429121748 | 5.1119215924331 | c   |
| 6.93443408839721 | 30.63643162173187 | 13.7964408363478 | c   |
| -2.46590259546941 | 34.2874436363222 | 8.3725346383923 | c   |
| -0.73196661440610 | 31.2813695447926 | 13.3205100943073 | c   |
| -0.39294732734577 | 32.1027761649005 | 5.7360856408058 | c   |
| -2.50890102072492 | 30.326532302446 | 3.7633445610545 | c   |
| 0.90166795088517 | 25.68157745109736 | 11.6473839870256 | c   |
| 9.76414965025097 | 34.0883429121748 | 5.1119215924331 | c   |
| 6.93443408839721 | 30.63643162173187 | 13.7964408363478 | c   |
| -2.46590259546941 | 34.2874436363222 | 8.3725346383923 | c   |
| -0.73196661440610 | 31.2813695447926 | 13.3205100943073 | c   |
| -0.39294732734577 | 32.1027761649005 | 5.7360856408058 | c   |
| -2.50890102072492 | 30.326532302446 | 3.7633445610545 | c   |
| 0.90166795088517 | 25.68157745109736 | 11.6473839870256 | c   |
| 9.76414965025097 | 34.0883429121748 | 5.1119215924331 | c   |
| 6.93443408839721 | 30.63643162173187 | 13.7964408363478 | c   |
| -2.46590259546941 | 34.2874436363222 | 8.3725346383923 | c   |
| -0.73196661440610 | 31.2813695447926 | 13.3205100943073 | c   |
| -0.39294732734577 | 32.1027761649005 | 5.7360856408058 | c   |
| -2.50890102072492 | 30.326532302446 | 3.7633445610545 | c   |
| 0.90166795088517 | 25.68157745109736 | 11.6473839870256 | c   |
| 9.76414965025097 | 34.0883429121748 | 5.1119215924331 | c   |
| 6.93443408839721 | 30.63643162173187 | 13.7964408363478 | c   |

S21
| X   | Y   | Z            | Label      |
|-----|-----|--------------|------------|
| 3.49981177495306 | 23.44445634133997 | -7.39509515441543 | c |
| 4.74492558205794 | 24.9468907721670 | -11.336783662373 | c |
| 3.07784909115711 | 25.3902487510548 | -9.23616940396200 | c |
| 5.42267026357777 | 21.80690440452086 | -8.34361716135960 | c |
| 6.18388146899894 | 22.6959947182385 | -10.8018726297332 | c |
| 14.1068464385533 | 22.73963304303554 | -8.37254972897102 | c |
| 12.37485268940373 | 26.39125021253378 | -13.79624083770708 | c |
| 12.03468499440309 | 27.37229250224246 | -9.1136781251168 | c |
| 14.15149377433863 | 19.38856417155867 | -7.1185129306388 | c |
| 7.74509799995011 | 21.21299571390001 | -12.6668087957638 | c |
| 13.30662849302046 | 21.52189049098325 | -9.8834973198750 | h |
| 16.19960211913733 | 22.76467998626000 | -8.65707448656180 | h |
| 13.77104619076743 | 21.75776447822636 | -6.54328804881610 | h |
| 10.7828915209898 | 26.44541936055016 | -14.53618118725797 | h |
| 13.14594210904959 | 26.5723001372892 | -14.19772011505705 | h |
| 12.48542481068224 | 23.72093791559618 | -13.46153831178392 | h |
| 11.48172274763860 | 31.59800666806969 | -3.73751551560475 | h |
| 13.93362860979722 | 32.84548783909764 | -5.70372698676995 | h |
| 10.69389994526273 | 33.32622027600343 | -6.5340508383150 | h |
| 14.40826806019041 | 24.66107008336164 | -3.34499658989639 | h |
| 16.06330195808659 | 27.58686778257594 | -3.64208733996583 | h |
| 12.995666906036122 | 27.54150689806309 | -2.2177969343173 | h |
| 9.54054592689281 | 32.77280945386260 | -10.6793832688609 | h |
| 12.40823756840517 | 32.3785601344655 | -12.42612289307014 | h |
| 9.65529423412737 | 30.62600776464196 | -13.29730877836431 | h |
| 1.21249119090819 | 24.69659971937627 | -4.17236553362502 | h |
| 0.15201570906195 | 21.85437319569697 | -5.65818985762620 | h |
| 2.87015749322719 | 21.80229078371068 | -3.65701348144949 | h |
| 6.50762671525161 | 26.19629832230803 | -14.8607788690513 | h |
| 3.17152460059521 | 25.70517604730137 | -15.06980653591218 | h |
| 4.37261174706075 | 28.4458595419916 | -13.50829403851535 | h |
| 1.52402248988915 | 29.08043770124173 | -10.23563314271564 | h |
| -0.78472290328724 | 26.634086092879 | -9.87760448082913 | h |
| 0.66592423412737 | 28.00027790394495 | -7.14404503208112 | h |
| 6.29684955618637 | 19.50752651925423 | -5.02082011256975 | h |
| 5.11299780278201 | 17.75609839116275 | -7.65532292571380 | h |
| 8.29665034277833 | 18.8821587938180 | -7.6826336293018 | h |
| 9.46460732088625 | 20.36522111568170 | -11.80864551074342 | h |
| 6.61804609992929 | 19.61155131963791 | -13.45254043153205 | h |
| 8.35860540566101 | 22.3789433475786 | -14.29590840873640 | h |

$$[	ext{Cp}_2\text{Sm}]_3\text{P}_3(\text{CpMo(CO)}_2)_3]$$ (3)

5.86276396534874 | 20.50821928861572 | -8.70470976566935 | sm |
4.81108104488443 | 12.1371124590364 | 6.22101584230850 | sm |
1.00687351416065 | 12.39097293758883 | -11.5613925626440 | mo |
0.10637057678853 | 17.6083679695423 | -1.11243974352394 | mo |
-1.57307211884386 | 11.78084268367441 | -7.35845591873187 | p |
| x         | y         | z         | p         | o         |
|-----------|-----------|-----------|-----------|-----------|
| -0.7193947089930 | 15.6444951790062 | -8.29238576536565 | p       |
| 2.19351620945109 | 17.16265604284390 | -5.51117831735467 | p       |
| 3.2063367113074 | 14.09972574620192 | -2.95721030888068 | p       |
| 0.758712041046711 | 10.90296060264007 | -4.01620853404825 | p       |
| 3.403128123350477 | 15.5290612205573 | 3.3339493505492 | o       |
| 5.28401090373420 | 16.42894664787532 | -11.09371561087676 | o       |
| 3.25571825909646 | 22.57886551395781 | -0.64844824778809 | o       |
| 3.72765861737410 | 14.74956531379268 | -11.18007185749183 | c       |
| 0.58337762997324 | 13.5682898234090 | -15.96248402651640 | c       |
| -1.68126288634990 | 14.28610016625258 | -14.8062456248256 | c       |
| 3.2063367113074 | 14.09972574620192 | -2.95721030888068 | p       |
| 0.758712041046711 | 10.90296060264007 | -4.01620853404825 | p       |
| 3.403128123350477 | 15.5290612205573 | 3.3339493505492 | o       |
| 5.28401090373420 | 16.42894664787532 | -11.09371561087676 | o       |
| 3.25571825909646 | 22.57886551395781 | -0.64844824778809 | o       |
| 3.72765861737410 | 14.74956531379268 | -11.18007185749183 | c       |
| 0.58337762997324 | 13.5682898234090 | -15.96248402651640 | c       |
| -1.68126288634990 | 14.28610016625258 | -14.8062456248256 | c       |
| 3.2063367113074 | 14.09972574620192 | -2.95721030888068 | p       |
| 0.758712041046711 | 10.90296060264007 | -4.01620853404825 | p       |
| 3.403128123350477 | 15.5290612205573 | 3.3339493505492 | o       |
| 5.28401090373420 | 16.42894664787532 | -11.09371561087676 | o       |
| 3.25571825909646 | 22.57886551395781 | -0.64844824778809 | o       |
| 3.72765861737410 | 14.74956531379268 | -11.18007185749183 | c       |
| 0.58337762997324 | 13.5682898234090 | -15.96248402651640 | c       |
| -1.68126288634990 | 14.28610016625258 | -14.8062456248256 | c       |
| x               | y               | z               |
|----------------|----------------|----------------|
| -2.158543      | 11.029430      | 6.351194       |
| -0.536737      | 8.071667       | 5.274311       |
| 3.314578       | 2.990087       | 7.858437       |
| 9.413144       | 5.274311       | 10.052902      |
| 9.615029       | 4.395930       | 7.159323       |
| 2.044067       | 0.937318       | 5.373621       |
| 9.526727       | 10.052902      | 5.346543       |
| 10.247916      | 10.052902      | 5.373621       |
| -0.214326      | 10.052902      | 5.346543       |
| -3.302084      | 10.052902      | 5.373621       |
| 3.314578       | 10.052902      | 5.346543       |
| 9.526727       | 10.052902      | 5.373621       |
| 10.247916      | 10.052902      | 5.346543       |
4.57063836339430 -0.31492935260766 -16.56756558069831 h
8.44936843312906 -2.8366075560224 -12.38834933978011 h
6.03202694643538 -5.1060028037441 -11.75526069339052 h
7.91211463925681 -3.91094246895998 -9.2229390227120 h
2.0135278924822 -14.50087833944642 -16.93885103478649 h
-2.2835301642015 16.26630080442016 -14.7125849718299 h
-4.83482979125085 12.25240903683237 -12.77271951097641 h
2.0806213845737 9.38896993146503 -16.43577120685265 h
-2.19702500472704 7.99664258148307 -13.88098840918734 h
-3.58138991267661 22.1634177231067 -1.52379837588259 h
-4.25941155353529 18.54379346895998 -5.1274273872180 h
-2.6344925074182 13.97217443699261 -2.82869795305392 h
-3.66823621268756 14.72855751478762 3.3234068259790 h
-2.8215572620229 4.9951145328016 14.9664827285874 h
-2.46198009758161 1.99759619551036 -0.82819156531254 h
-4.21443494788395 4.66862600172051 -4.8868094609385 h
-5.55758678767956 9.32672621461028 -3.25315453837616 h
-4.78951363890673 9.45011513561381 1.82897329034571 h
3.4723887886657 9.92304870446174 14.9968428725874 h
6.27408206977958 11.41359462047031 3.84389638410373 h
5.4778293321902 8.82677801149004 12.8287841712478 h
2.44993862447961 16.59700538741467 13.8263972539700 h
4.03775692171138 17.81553119741853 11.10901546186286 h
5.60331032640201 15.60201655570437 13.13070010661522 h
0.77391257956731 18.20764731751627 8.10341901276195 h
-2.13670172272779 17.03761572382374 9.36502856402014 h
-1.32465242547905 16.44578216859751 6.130299659660 h
-1.80928145967207 11.6830706309947 4.38187325030383 h
-3.95994477898433 11.9160063923433 6.8981797155006 h
-2.48718981952801 8.96122419522905 6.24870201535622 h
2.9096156002025 6.05200162448075 10.19045283574373 h
0.86395482831883 6.29520352498225 7.5104309777522 h
-0.41866327866358 6.38810684692070 10.6418600066909 h
9.72087893663448 14.16199147503944 11.9354250815594 h
9.21814310636007 16.91359608200773 10.0323773935624 h
12.28561645303285 15.51635123071425 10.2026307360392 h
9.94365560180705 9.91932980908928 11.90261997366834 h
9.12742369930024 7.20398840616811 10.0591882604274 h
12.2776836528409 8.40984202284229 9.8399295817176 h
8.60387702347643 17.28381196407483 2.63315801460206 h
11.65863747605181 17.50913711369817 4.06612432447369 h
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| X    | Y    | Z    | h     |
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| 8.47080347751787   | 26.95865722397134 | -12.49343112182945 | h     |
| 8.02624045367683   | 27.94306505597820 | -9.28369220253196 | h     |
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| 11.08139350831705  | 4.47952837430000 | -1.25874480138556 | h     |
| 7.99097242782069   | 5.76586760750291 | -1.76082823427631 | h     |

\[\text{[\{CpMo(CO)\_2\}_2(\mu-\eta^2-P_2)\]}\]
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-5.79697181476800  -2.43138898495034  -0.51452909616275  o
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-4.07483525433803  3.78130365325948  -0.49707393823989  c
-2.63282310796967  2.78370115167377  -2.5680943316993 c
-0.5687739286940  4.46519268262623  -3.04344145108126  c
-0.72896813762676  6.52593385655267  -1.28266027556845 c
-3.59768525219779  7.34489165299907  1.79834979349223 h
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-3.08128229182976  1.06870125326766  -3.64033247559632 h
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