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
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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 $LiAlH_4$. Tetrahydrofuran was distilled under nitrogen from potassium benzophenone ketyl before storage over $LiAlH_4$. 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] $[\{CpMo(CO)_2\}_2(\mu,\eta^{2:2}\text{-}P_2)]$,[4] and $[Cp^*Mo(CO)_2(\eta^3\text{-}P_3)]$[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 CaF_2 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.

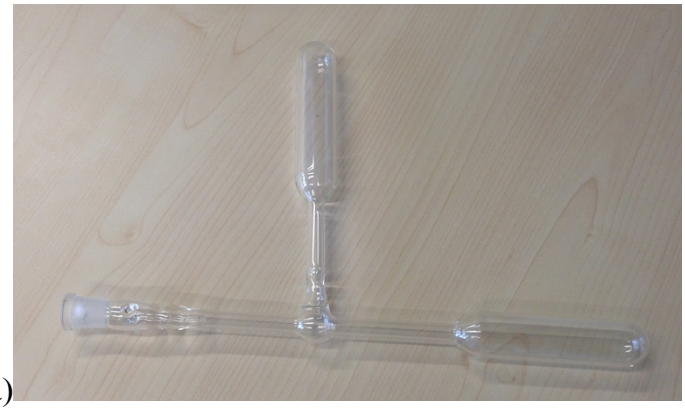
a)  b) 

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

[(Cp*$_2$Sm)$_2$P$_2$(CpMo(CO)$_2$)$_4$] (1a)

In a three-section-ampoule, toluene (15 mL) was condensed at -78 °C onto a mixture of [Cp*$_2$Sm(thf)$_2$] (80 mg, 0.14 mmol) and [{CpMo(CO)$_2$}$_2$(μ,η$^{2:2}$-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 [(Cp*$_2$Sm)$_2$P$_2$(CpMo(CO)$_2$)$_4$] were obtained. The supernatant solution was decanted and the section with [(Cp*$_2$Sm)$_2$P$_2$(CpMo(CO)$_2$)$_4$] was flamed-sealed. Yield: 10 mg, 7 % (single crystals).

IR (ATR, $\tilde{\nu}$/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, $\tilde{\nu}$/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 $C_{68}H_{80}Mo_4O_8P_2Sm_2$ (1771.89 g·mol^{-1}) (**1** – 1 Tol): C, 46.09; H, 4.55. Found: C, 46.01; H, 4.32.

[(Cp*$_2$Sm)$_2$P$_4$(CpMo(CO)$_2$)$_2$] (2) and [(Cp*$_2$Sm)$_3$P$_5$(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*$_2$Yb)$_2$P$_2$(CpMo(CO)$_2$)$_4$] (1b)

In a two-section ampoule, toluene (15 mL) was condensed at -78 °C onto a mixture of [Cp*$_2$Yb(thf)$_2$] (82 mg, 0.14 mmol) and [{CpMo(CO)$_2$}$_2$(μ,η$^{2:2}$-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, crystals of [(Cp*$_2$Yb)$_2$(CpMo(CO)$_2$)$_4$P$_2$] were obtained. Yield: 8 mg, 6 % (single crystals).

IR (ATR, $\tilde{\nu}$/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 $C_{68}H_{80}Mo_4O_8P_2Yb_2$ (1817.10 g·mol^{-1}): C, 44.49; H, 4.44. Found: C, 44.76; H, 4.27.

[(Cp*$_2$Sm)$_2$P$_6$(Cp*Mo(CO)$_2$)$_2$] (4)

Toluene (15 mL) was condensed at -78 °C onto a mixture of [Cp*$_2$Sm(thf)$_2$] (178 mg, 0.316 mmol) and [Cp*Mo(CO)$_2$(η^3-P$_3$)] (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*$_2$Sm)$_2$P$_6$(Cp*Mo(CO)$_2$)$_2$] were obtained. Yield: 20 mg, 14 % (single crystals).

IR (ATR, $\tilde{\nu}$/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, $\tilde{\nu}$/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 $C_{71}H_{98}Mo_2O_4P_6Sm_2$ (1694.04 g·mol^{-1}) (**4** – 1Tol): C, 50.34; H, 5.83. Found: C, 50.46; H, 6.02.

[(Cp*$_2$Yb)$_2$P$_6$(Cp*Mo(CO)$_2$)$_2$] (5)

Toluene (15 mL) was condensed at -78 °C onto a mixture of [Cp*$_2$Yb(thf)$_2$] (157 mg, 0.273 mmol) and [Cp*Mo(CO)$_2$(η^3-P$_3$)] (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*$_2$Yb)$_2$P$_6$(Cp*Mo(CO)$_2$)$_2$] were obtained. Yield: 14 mg, 18 % (single crystals). IR (ATR, $\tilde{\nu}$/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 $C_{67}H_{94}Mo_2O_4P_6Yb_2$ (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.[6] 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 $(F_o\text{-}F_c)^2$, where the weight is defined as $4F_0^2/2(F_o^2)$ and F_o and F_c are the observed and calculated structure factor amplitudes using the program SHELXL-2013.[6] 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**: $C_{68}H_{80}Mo_4O_8P_2Sm_2 \bullet C_7H_8$, M = 1863.85, a = 9.5023(3) Å, b = 12.6103(4) Å, c = 15.1418(5) Å, α = 97.784(3)°, β = 90.790(3)°, γ = 100.069(3)°, V = 1768.68(10) Å^3, T = 100 K, space group P-1, Z = 1, 17149 reflections measured, 6969 independent reflections (R_{int} = 0.0684). The final R_1 values were 0.0516 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1266 ($I > 2\sigma(I)$). The final R_1 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**: $C_{68}H_{80}Mo_4O_8P_2Yb_2$, M = 1817.10, a = 9.4563(7) Å, b = 12.5189(13) Å, c = 14.9787(13) Å, α = 84.903(8)°, β = 71.669(7)°, γ = 76.285(7)°, V = 1635.0(3) Å^3, T = 150 K, space group P-1, Z = 1, 14805 reflections measured, 5918 independent reflections (R_{int} = 0.0698). The final R_1 values were 0.0392 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0708 ($I > 2\sigma(I)$). The final R_1 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**: $C_{54}H_{70}Mo_2O_4P_4Sm_2 \bullet 2(C_7H_8)$, M = 1583.82, a = 9.6185(7) Å, b = 10.2667(7) Å, c = 17.5096(13) Å, α = 83.519(6)°, β = 77.307(6)°, γ = 78.461(6)°, V = 1648.44(21) Å^3, T = 100 K, space group P-1, Z = 1, 12256 reflections measured, 5964 independent reflections (R_{int} = 0.1155). The final R_1 values were 0.0708 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1908 ($I >$

$2\sigma(I)$). The final R_1 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**: $C_{81}H_{105}Mo_3O_6P_5Sm_3$, M = 2068.36, a = 10.130(2) Å, b = 25.686(5) Å, c = 15.724(3) Å, α = 90°, β = 96.36(3)°, γ = 90°, V = 4066.3(14) Å^3, T = 100 K, space group $P121/m1$, Z = 2, 33852 reflections measured, 7394 independent reflections (R_{int} = 0.2911). The final R_1 values were 0.1092 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.2500 ($I > 2\sigma(I)$). The final R_1 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**: $C_{64}H_{90}Mo_2O_4P_6Sm_2 \bullet 2(C_7H_8)$, M = 1786.02, a = 11.1671(8) Å, b = 12.7931(10) Å, c = 14.7276(9) Å, α = 98.952(6)°, β = 110.227(6)°, γ = 95.319(6)°, V = 1925.7(2) Å^3, T = 123 K, space group P-1, Z = 1, 15246 reflections measured, 6698 independent reflections (R_{int} = 0.0368). The final R_1 values were 0.0343 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0799 ($I > 2\sigma(I)$). The final R_1 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 1.066.

Crystal data for **5**: $C_{64}H_{90}Mo_2O_4P_6Yb_2 \bullet 2(C_7H_8)$, M = 1831.40, a = 11.1924(3) Å, b = 12.6285(3) Å, c = 14.6371(4) Å, α = 99.581(2)°, β = 110.455(2)°, γ = 94.847(2)°, V = 1888.44(9) Å^3, T = 100 K, space group P-1, Z = 1, 17122 reflections measured, 7340 independent reflections (R_{int} = 0.0260). The final R_1 values were 0.0410 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1014 ($I > 2\sigma(I)$). The final R_1 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**.

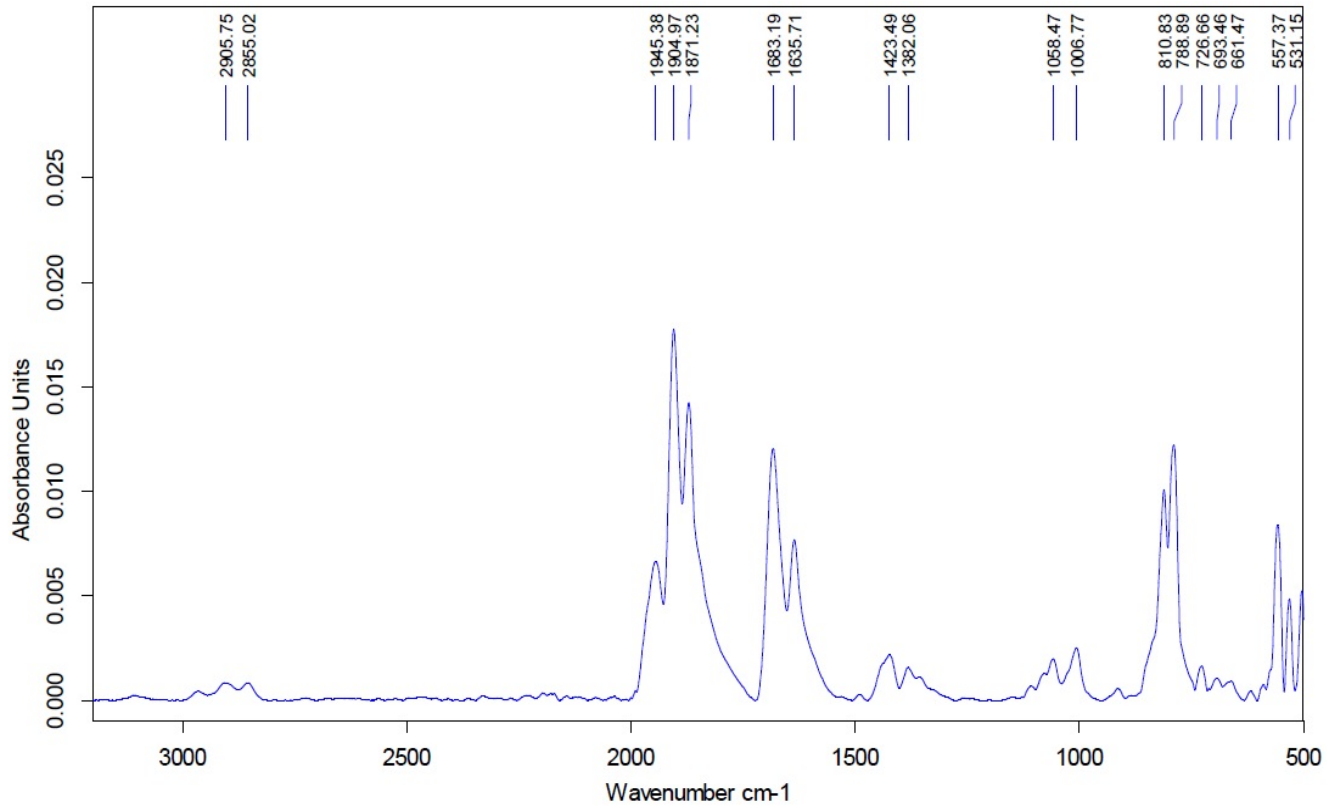


Figure S3. NIR-spectrum of **1a**.

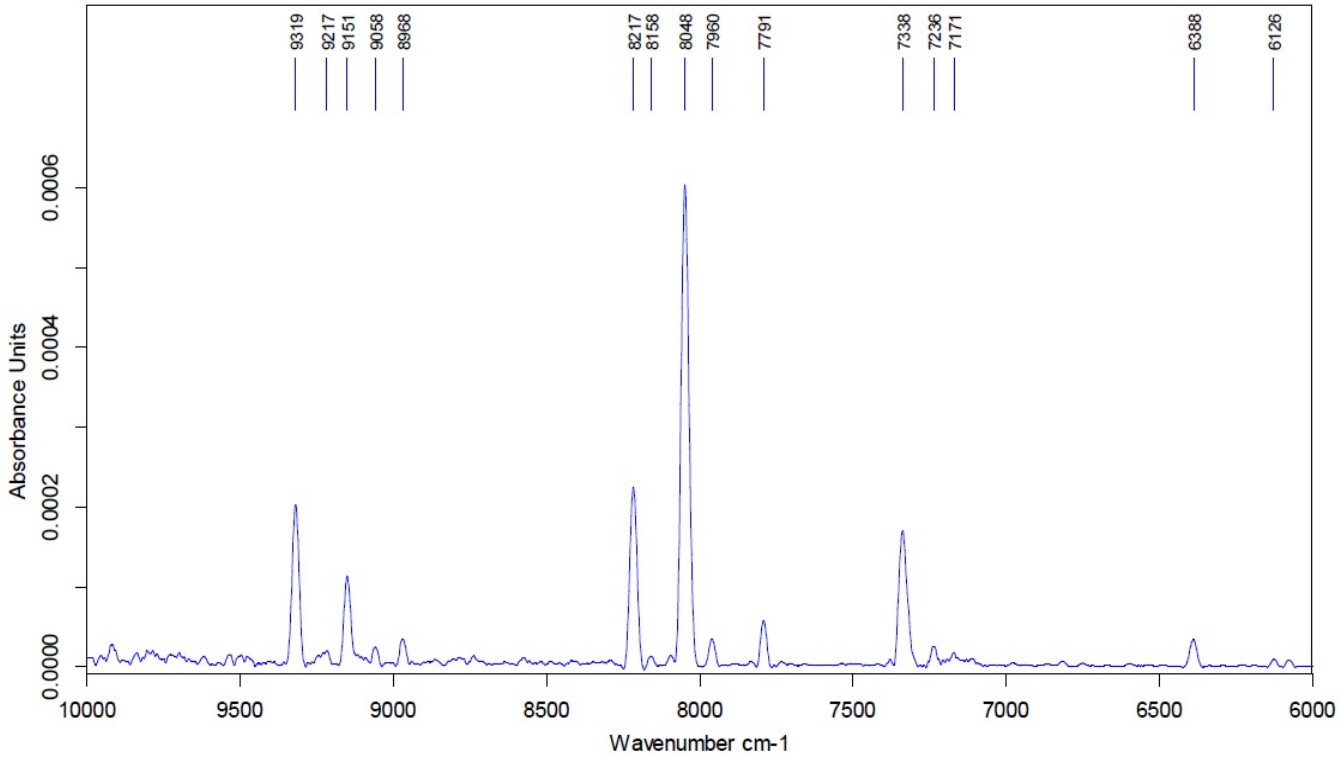


Figure S4. IR-spectrum of **1b**.

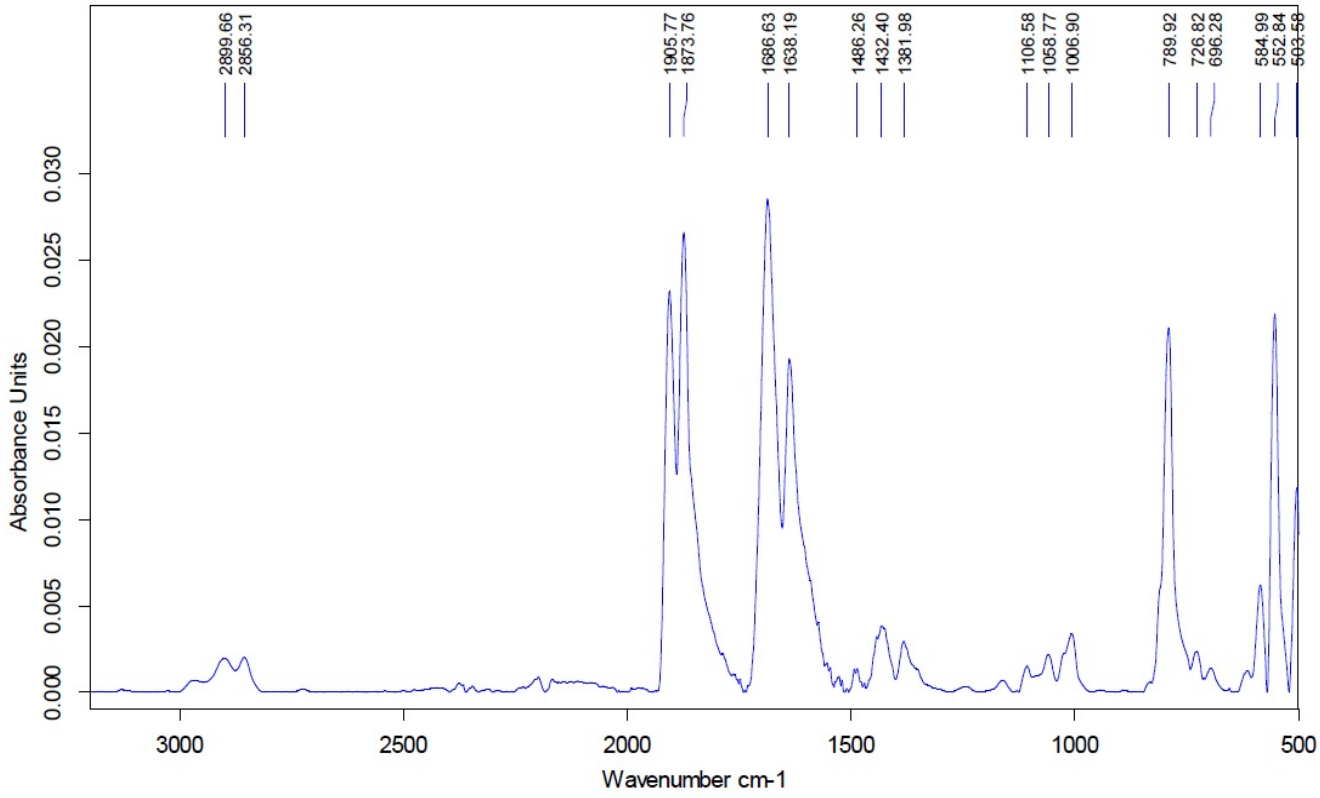


Figure S5. Solid-state structure of **3** showing the full disordered of the central P_5-core. Hydrogen atoms are omitted for clarity.

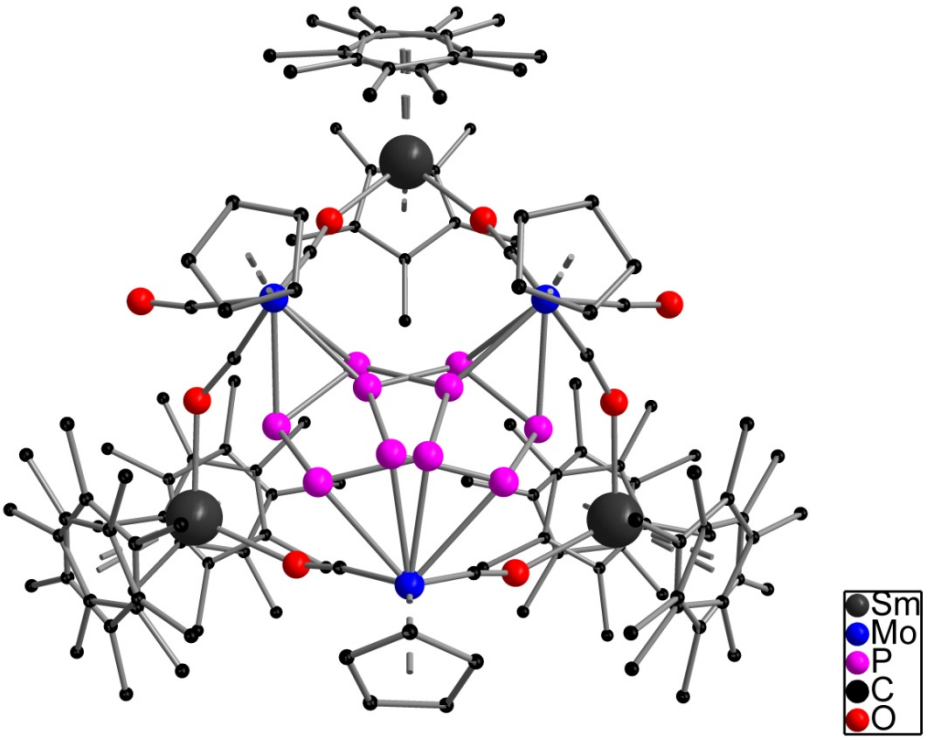


Figure S6. Solid-state structure of **3** showing each part of the disordered structure separated.

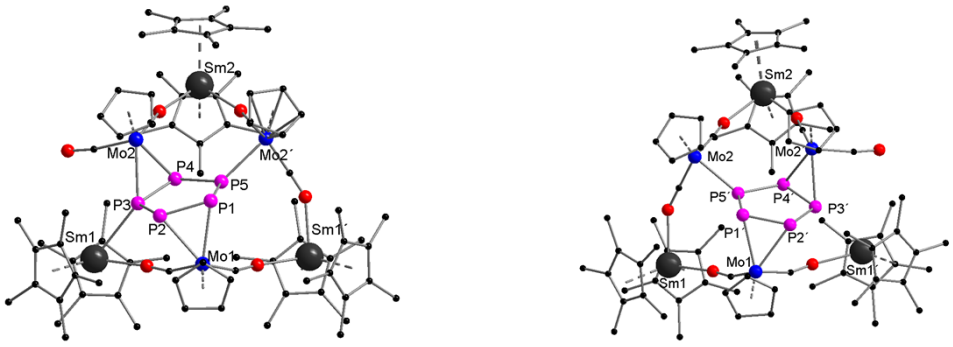


Figure S7. Solid-state structure of **4** showing the full disordered of the central P_6-core. Hydrogen atoms are omitted for clarity.

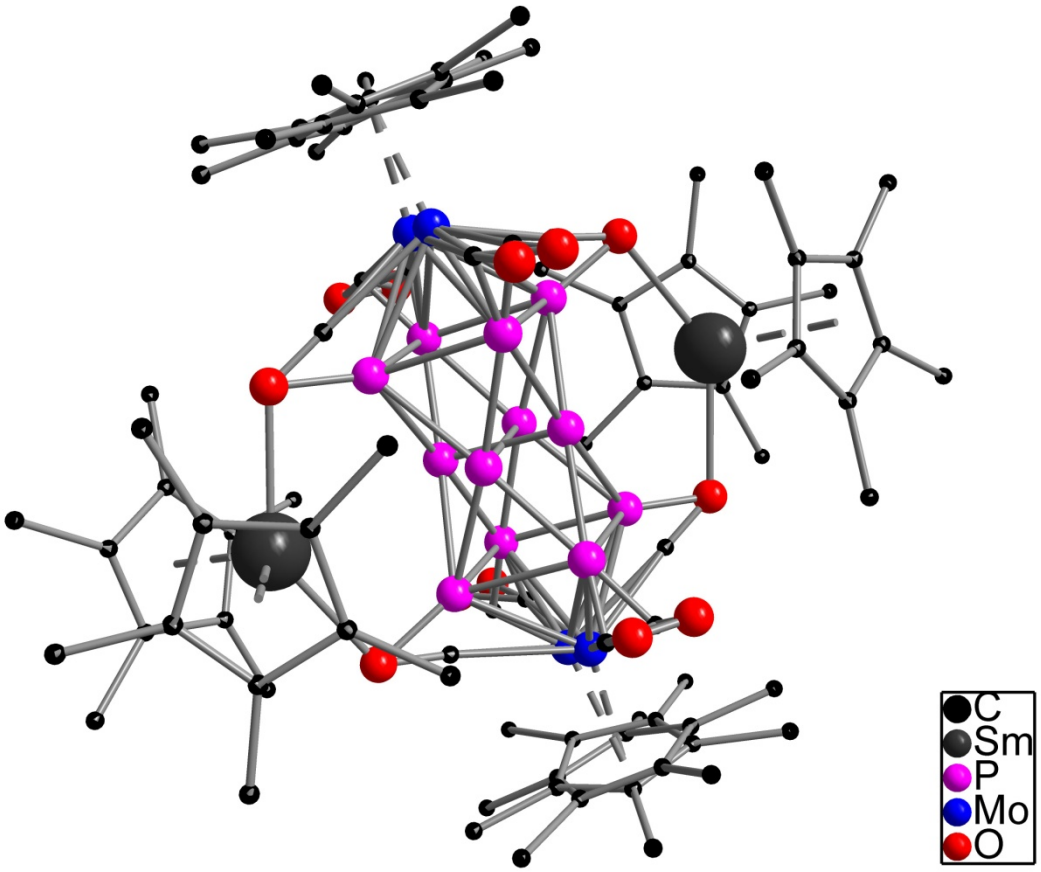


Figure S8. Solid-state structure of **4** showing the four-fold disordering of the central P_6-core only.

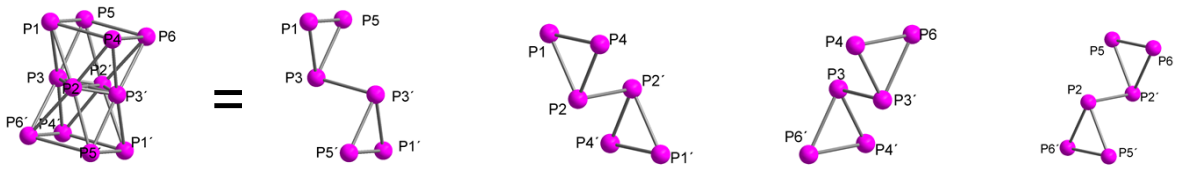
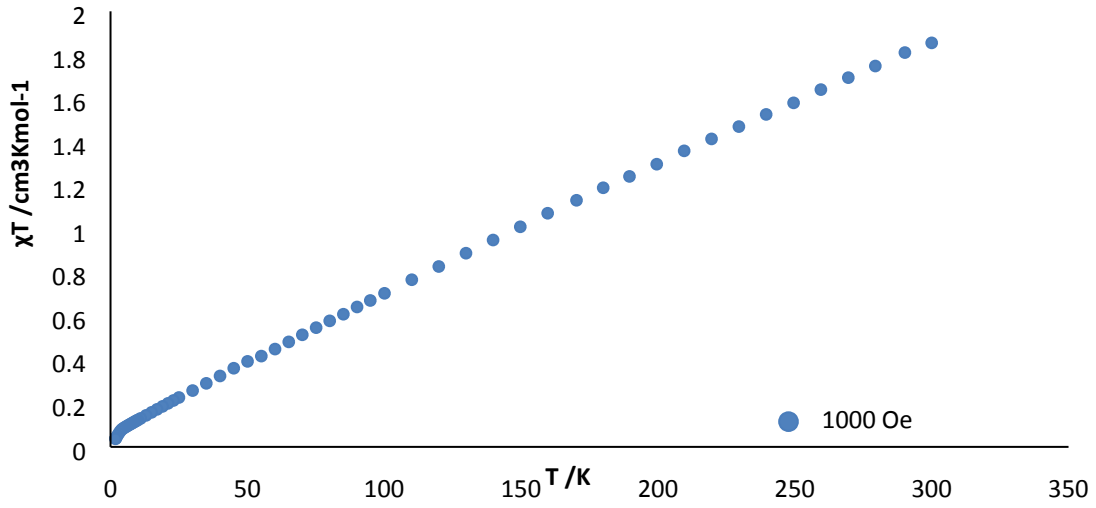


Figure S9. Temperature-dependent SQUID magnetization data for **4**. $\chi_M T$ versus T plot at 1000 Oe and M versus T plot.



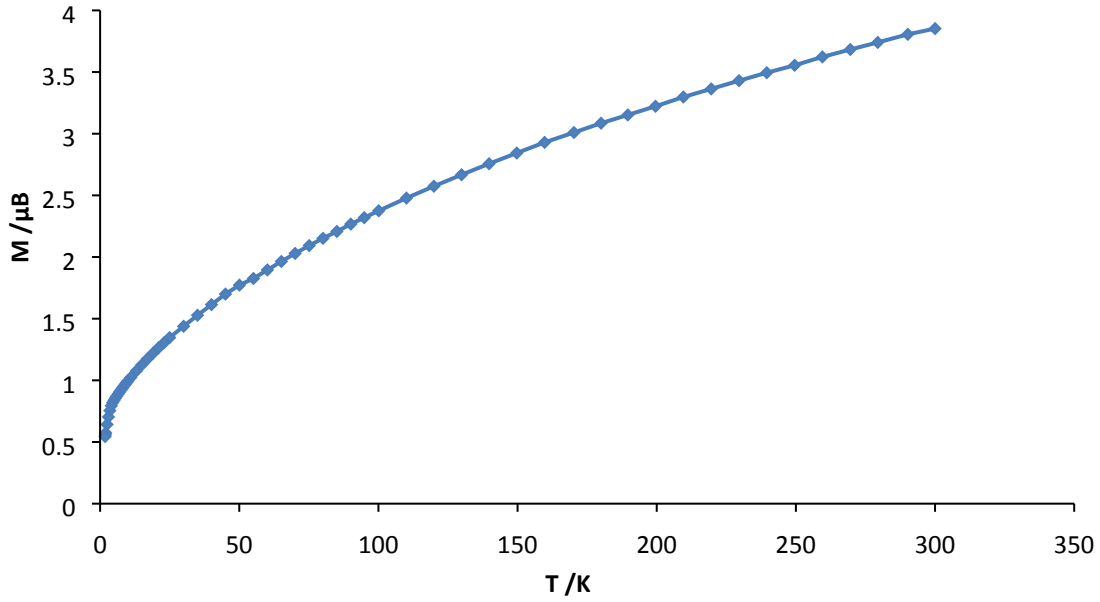


Figure S10. IR-spectrum of **4**.

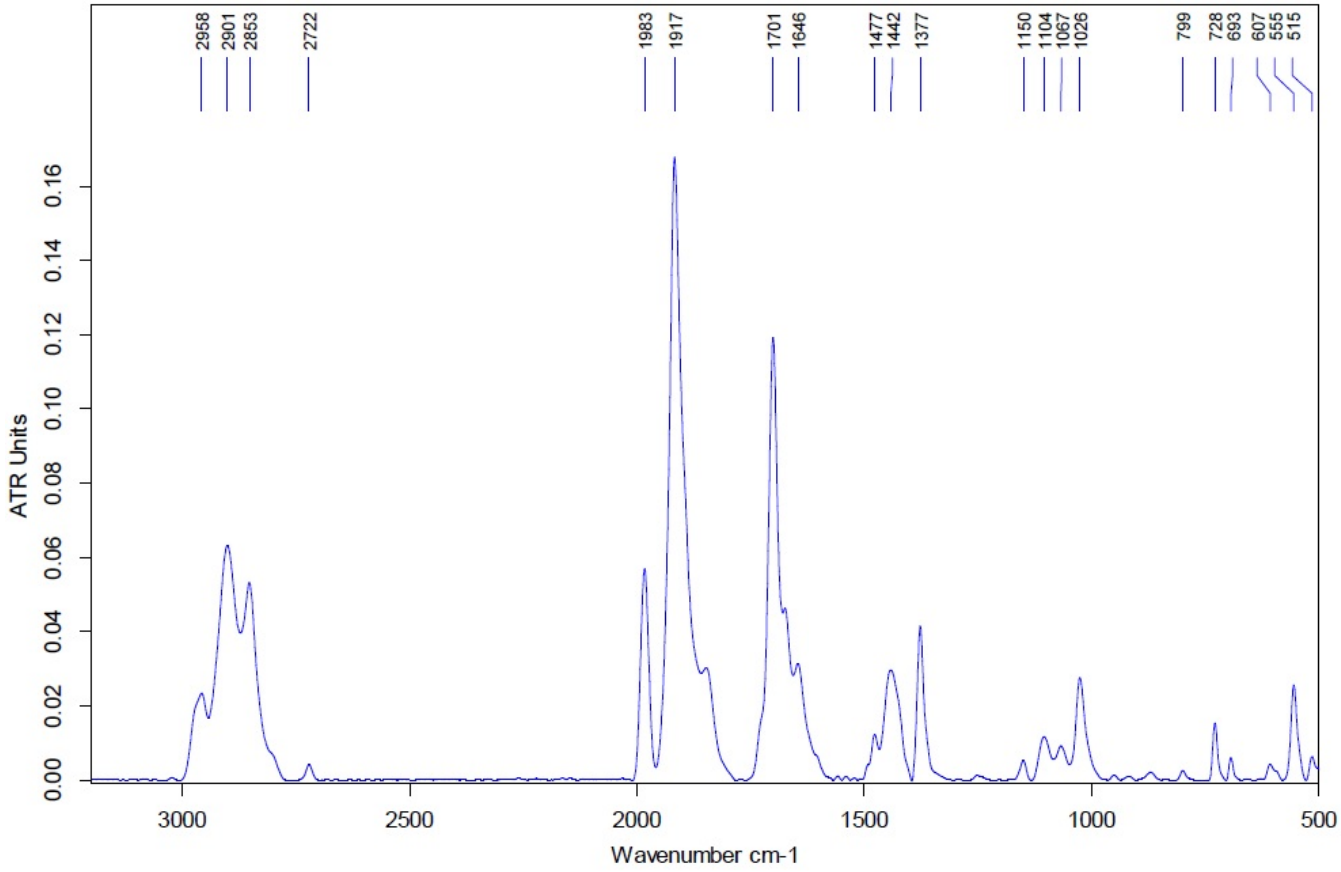


Figure S11. NIR-spectrum of **4**.

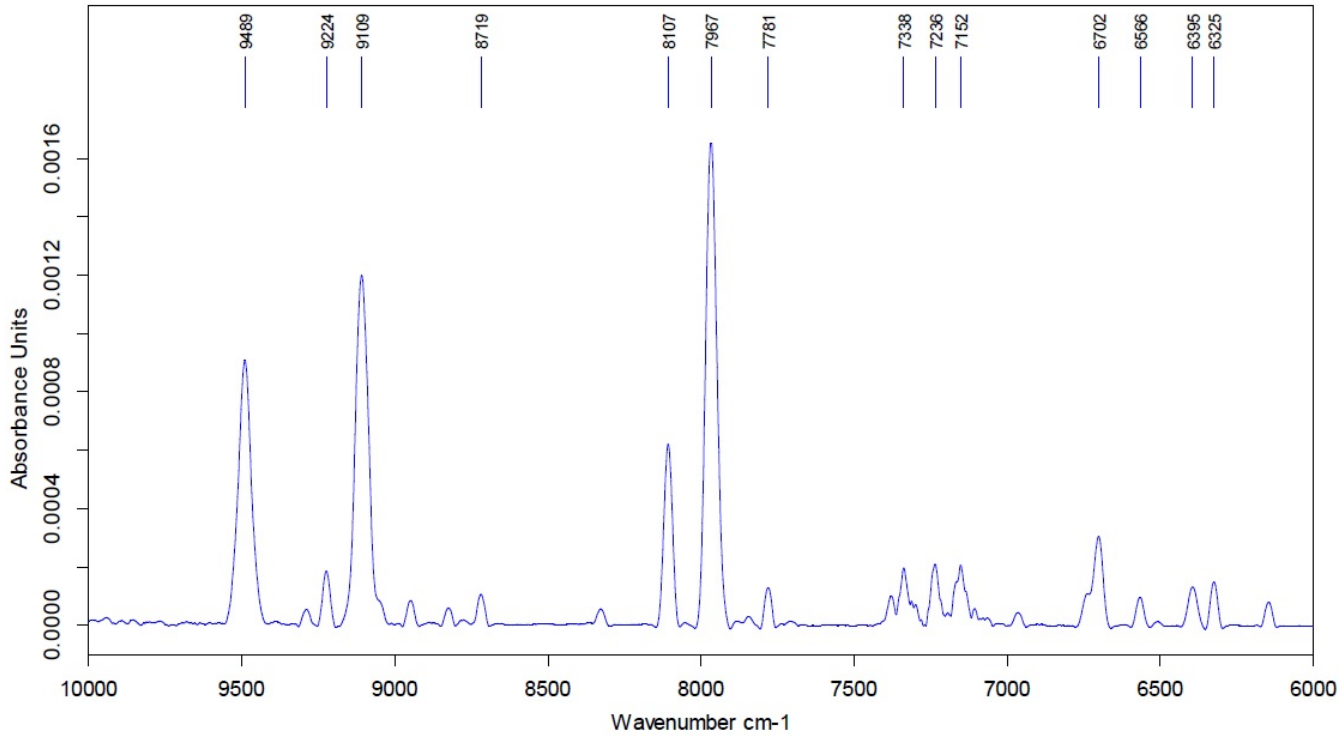
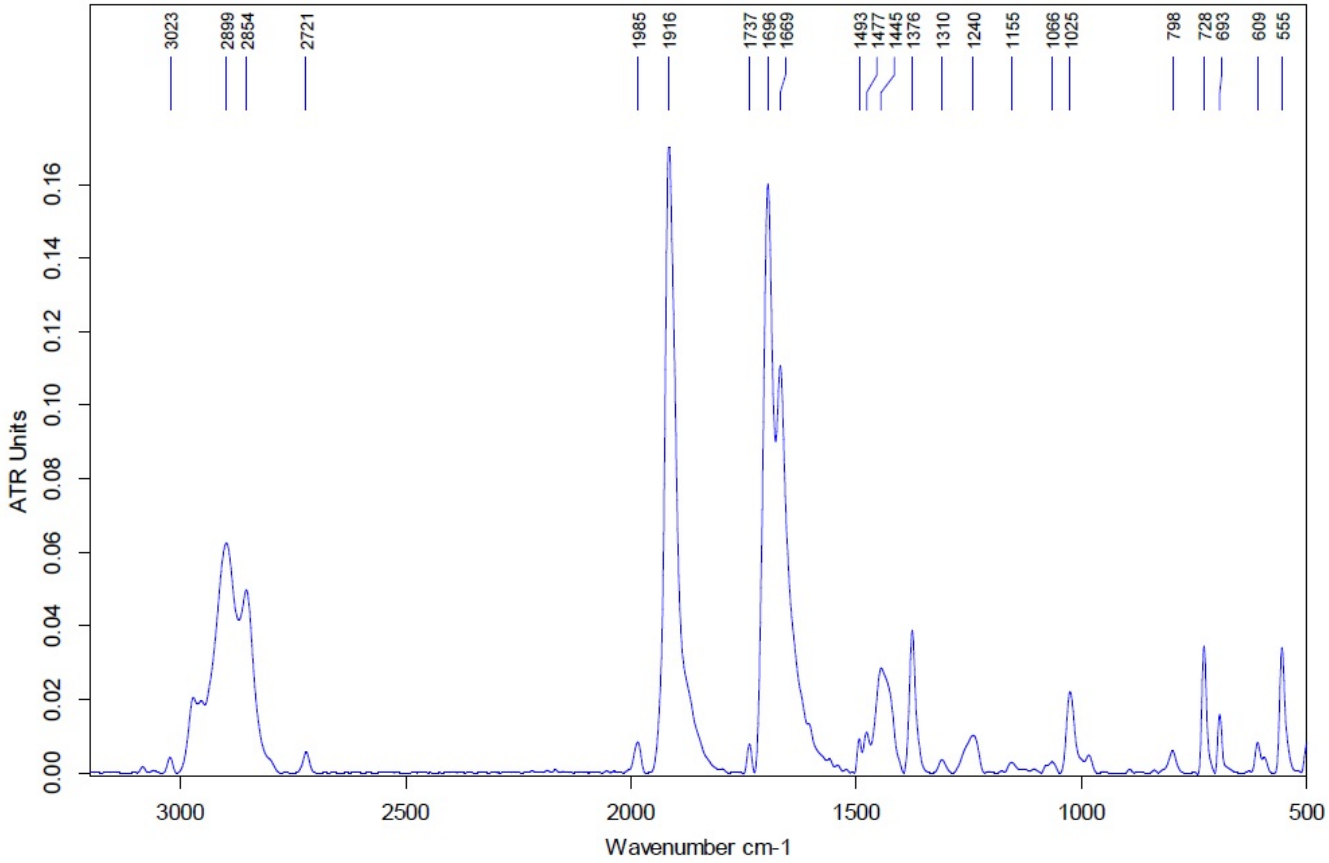


Figure S12. IR-spectrum of **5**.



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 [{$CpMo(CO)_2$}$_2$($\mu,\eta^{2:2}$-P_2)].

	[$(Cp_2$*Ln$)_2P_2$ ($CpMo(CO)_2)_4$]	[$(Cp^*_2Sm)_2P_4$ ($CpMo(CO)_2)_2$]	[$(Cp^*_2Sm)_3P_5$ ($CpMo(CO)_2)_3$]	[{$CpMo(CO)_2$}$_2$($\mu,\eta^{2:2}$-P_2)]
	1a	**2**	**3**	
r(P-P)	2.078	2.181 (P1-P2, P1'-P2'), 2.328 (P1-P2', P1'-P2)	2.205 (P1-P5, P4-P5), 2.151 (P3-P4), 2.174 (P1-P2), 2.278 (P2-P3)	2.121
r(Mo-P)	2.406	2.568 (Mo'-P1', Mo-P1) 2.588 (Mo-P1', Mo'-P1)	2.394 (Mo2'-P5) 2.663 (Mo2-P4) 2.630 (Mo1-P1) 2.587 (Mo2-P3) 2.606 (Mo1-P2)	2.505
r(Mo-Mo)	3.247			3.087
SEN(P-P)	1.38	1.24 (P1-P2, P1'-P2'), 0.98 (P1-P2', P1'-P2)	1.12 (P1-P5, P4-P5), 1.24 (P3-P4), 1.30 (P1-P2), 1.04 (P2-P3)	1.41
SEN(Mo-P)	0.77	0.59	0.66 (Mo2'-P5) 0.53 (Mo2-P4) 0.43 (Mo1-P1) 0.61 (Mo2-P3) 0.54 (Mo1-P2)	0.55
SEN(Mo-Mo)	0.23			0.30
SEN(Sm-P)			0.74 (Sm1-P3)	
Q(Sm)	1.04	0.38	Sm1: 0.35 Sm1': 1.21 Sm2: 1.10	
Q(Mo)	-0.52	-0.52	Mo1: -0.45 Mo2: -0.55 Mo2': -0.41	-0.54
Q(P)	0.02	0.03	P1: -0.20 P2: -0.08 P3: 0.00 P4: -0.01 P5: -0.08	0.07

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 $Na_4P_2^{2+}$, Na_2P_4, NaP_5 and $Na_3P_5^{2+}$ as well as T_d- and D_{2h}-P_4.

	$Na_4P_2^{2+}$	Na_2P_4	NaP_5	$Na_3P_5^{2+}$	P_4	P_4
symmetry	D_{2h}	D_{4h}	C_{5v}	C_s	T_d	D_{2h}
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		
Q(P)	-0.12	-0.20	-0.11	-0.01	0.00	0.00

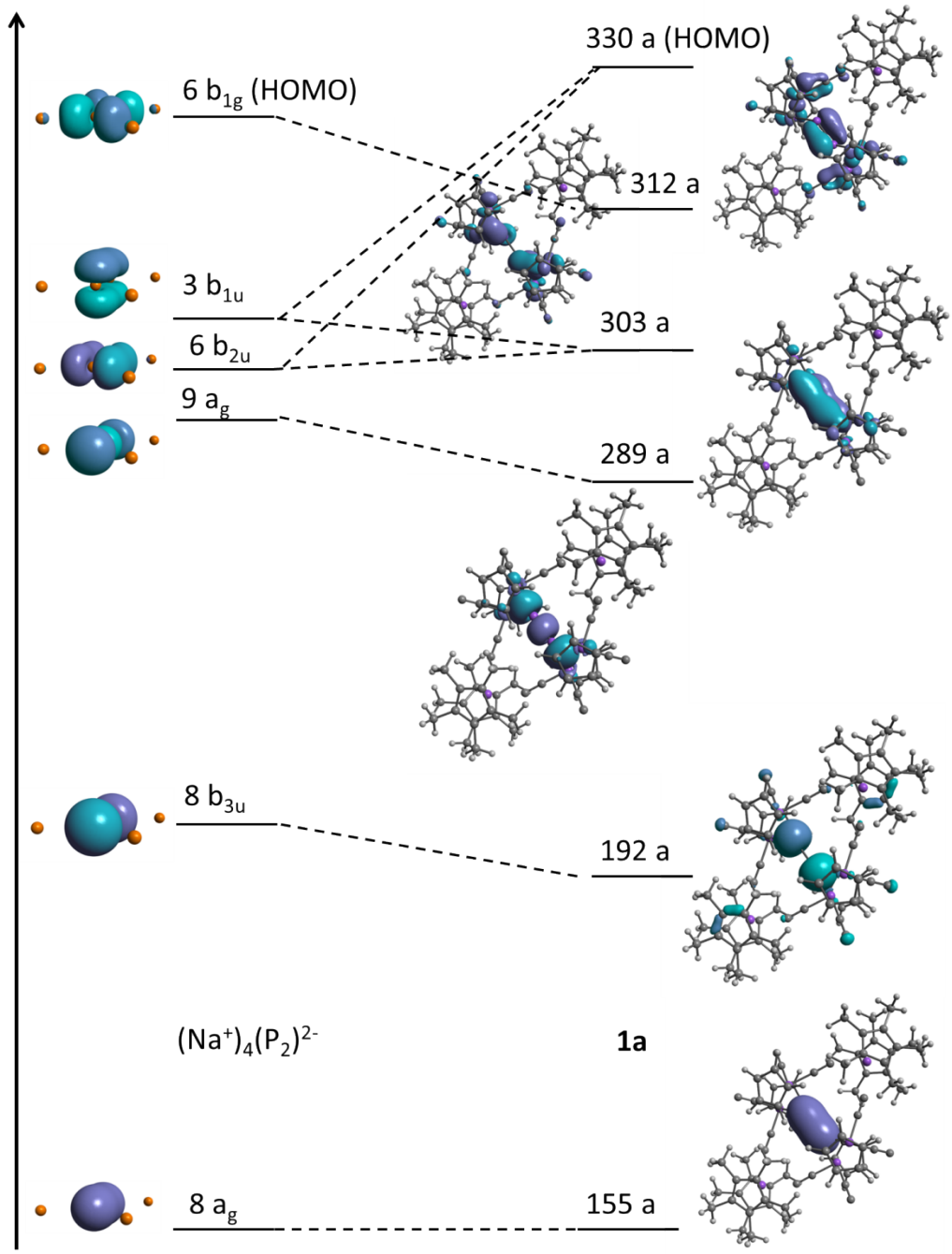


Figure S13: Comparison of the MO diagrams of $Na_4P_2^{2+}$ and $[(Cp_2^*Ln)_2P_2(CpMo(CO)_2)_4]$. Only the MOs with strong phosphorus contribution are shown.

Cartesian Coordinates of the calculated Molecules (given in a.u.)

$[(Cp_2{*}Ln)_2P_2(CpMo(CO)_2)_4]$ (**1a**)

1.90296250200252	-13.82810402990115	8.09534720152958	h
0.08122360005252	-14.84040850928407	10.74781306916709	h
1.37981219598989	-13.32253036468599	10.06893260714207	c
0.14023700628127	-10.76210982108238	10.25462714082543	c
3.12034011868955	-13.44567223958481	11.22950563951258	h
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-1.79623458133009	-9.84804709039902	8.58549018910282	c
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6.82253254791578	-5.76266175750081	10.33650701072655	c
6.58097664707015	-3.74159490644463	8.53832573999748	c
1.83565304463779	-9.42455544331244	14.72432686216367	c
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-0.25732801015706	-6.08500904503992	1.71864829632883	c
-0.29226672059125	-0.25195397447684	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
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6.58115131985332	-0.96191815085404	9.15814758903328	c
3.55942517508755	-10.58232404058777	14.41696181079272	h
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-3.63426123703807	-9.91965274821820	4.89291852001703	h
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-1.34427270025411	-12.36323561746168	5.33458984730631	h
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-3.48030741710567	-5.34959258230432	15.07890028353203	h
-2.58659666915900	-3.10994889237606	12.70622496804775	h
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-0.37336578120060	-1.32658613395400	-1.39778186147951	p
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-5.93474374175377	0.78423625099102	5.64824892736753	c
-5.98873817891798	2.04326321832465	3.25311600627792	c
-5.68901988945465	4.69548968816598	3.69117336133280	c
-5.41236288820401	5.08229006229943	6.35371190113451	c
-5.58209716311298	2.66522472421912	7.57857496158817	c
1.86926100357004	-2.54829277181908	-5.16242235255147	mo
2.02944698171460	-9.62641149298908	-3.27165512492342	o
-5.72360801700738	-4.35436413048413	-5.91987541741338	h
-4.54310671283884	-9.28151231298895	-5.16670795392077	h
-5.02629672794088	-10.29846838145748	-0.12931314263630	h
-6.45821912767175	-5.93180734092210	2.22340945235708	h
-6.89276290639923	-2.27003143806304	-1.36757853678393	h
1.91625972857264	5.60240500095467	1.42106562103362	mo
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-6.17626447278180	-1.25107508569177	5.95957150201203	h
-6.22614812457104	1.13745580473912	1.40487390580314	h
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-1.57179220114653	-5.76056838430821	-8.78212473148298	o

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5.65915712896344	-6.18192817510887	-2.24682670013210	h
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5.53193540433425	-2.32894590646508	-9.62549420250546	h
-0.74257997887000	6.52406958430247	-3.74242620292511	o
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4.64066896627686	22.40228518809662	1.61978178874903	c
6.52968710989899	25.53319691493463	4.94649241275463	c
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14.15149377433863	26.70077740531456	-3.76306316817857	c
10.74100377025894	31.34584655601239	-11.64753923005731	c
1.87873918868486	22.93892759618083	-5.11224809854494	c
4.70855628931678	26.39125201253378	-13.79692408387708	c
1.03745899896233	27.37322950224246	-9.11336781251168	c
6.33793817311596	19.38856417155867	-7.11851255903688	c
7.74509879999501	21.21299571319001	-12.66680897597638	c
13.30662849302046	21.52189049098325	-9.88349733198750	h
16.19960521191373	22.76467998626000	-8.65707448656180	h
13.77104619076743	21.75776447822636	-6.54328804881610	h
10.78282915209897	26.44541936305616	-14.53618118725797	h
14.13594121909459	26.57253001372892	-14.19720115057059	h
12.48542481068224	23.72093791559618	-13.46153831178392	h
11.48172274763860	31.59800069860697	-3.73751551560475	h
13.93362069799722	32.84548783909764	-5.70372698676995	h
10.69389994526273	33.32622027600343	-6.53405080383150	h
14.40826806019041	24.66107008336614	-3.34499695898693	h
16.06330195808659	27.58686778257594	-3.64208733996583	h
12.99566690361322	27.54150689806039	-2.21779693343173	h
9.54054592689281	32.77280945382620	-10.67993832688609	h
12.40823756840517	32.37856011344655	-12.42612289307014	h
9.65529423412737	30.62600776461496	-13.29730877836431	h
1.21214911090819	24.69659971937627	-4.17236653362502	h
0.15201570906195	21.85437319569697	-5.65818985726620	h
2.87015749322719	21.80229078371068	-3.65701348144949	h
6.50762671527516	26.19629832230803	-14.86077886890513	h
3.17152460059521	25.70517604730137	-15.06980653591218	h
4.37261174706075	28.44658955419916	-13.50829403851535	h
1.52402248988915	29.08043770124173	-10.23563314271564	h
-0.78472290328724	26.63408600928795	-9.87760448082913	h
0.66592422872995	28.00277903944955	-7.14404503208112	h
6.29684955618637	19.50752651925423	-5.02082011256975	h
5.11299780272801	17.75609839116275	-7.65532292571380	h
8.29665034277833	18.88271587938180	-7.68826336293018	h
9.46640732088625	20.36522111568170	-11.80864551074342	h
6.61804600992929	19.61155131963791	-13.45254043153205	h
8.35860540566101	22.37879433475876	-14.29590840873640	h

[$(Cp^*_2Sm)_3P_5(CpMo(CO)_2)_3$] (**3**)

5.86276396534874	20.50821928861572	-8.70470976566935	sm
4.81108104488443	12.13711245990364	6.22101584230850	sm
1.00687351416065	12.39097293758883	-11.56139259626440	mo
0.10637057678853	17.60836759695423	-1.11243974352394	mo
-1.57307211884386	11.78084268367441	-7.35845591873187	p

-0.71993947089930	15.64449517900626	-8.29238576536565	p
2.19351620945109	17.16265604284390	-5.51117831735467	p
3.20633637113074	14.09972574620192	-2.95721030888068	p
0.75871210467511	10.90296060264007	-4.01620853404825	p
3.40312128350477	15.52590612205573	3.33349943505492	o
5.28401090373420	16.42894664787532	-11.09371561087676	o
3.25571825909646	22.57886551395781	-0.64844842778809	o
3.72765681737410	14.74956531379268	-11.18007185749183	c
0.58337769297324	13.35682898234090	-15.96248402651640	c
-1.68126288634990	14.28610016625528	-14.80624546248256	c
-3.02325303651028	12.17102329373776	-13.78428515673283	c
-3.44433675040593	18.88040817643606	1.20642578901572	c
-3.65767213600868	20.11469919968086	-1.20079937677309	c
-4.02486233302451	18.22007868550421	-3.09123365898618	c
-4.03598259668340	15.80044583371159	-1.87585355342353	c
-3.68664814475826	16.20250459871628	0.77571457353169	c
2.19014044331269	16.35555689907498	1.57642889213336	c
9.34080643311420	12.07290381284729	3.69303118813330	c
9.46233492849165	14.25916028622119	5.30083600893110	c
9.64101697957336	13.40746708678402	7.87490547950089	c
9.35456612841897	12.10050599368418	0.84688280548678	c
9.65157497970633	16.96256939042446	4.42159702889781	c
10.22472095468429	15.07221964056871	10.11210588796176	c
1.46814196534365	23.34472911384144	-9.28482736488573	c
2.04027412600387	22.39508668221103	-11.76092860982654	c
4.32218092028681	23.59590139491578	-12.61913607097348	c
5.11748804902596	25.34972240717855	-10.69809355915762	c
3.39230581066577	25.14606711245356	-8.61320570713107	c
0.37796124844230	20.70573414687766	-13.33231639501469	c
5.46140700512055	23.31311746390824	-15.21959314796506	c
7.02293791180447	27.43433366599233	-11.05585624926613	c
3.34340641734328	26.80372739370885	-6.29173514938643	c
-0.92538202698957	22.90486876200530	-7.80739648268219	c
9.59390465584543	19.87421195024257	-5.15954045702562	c
10.17168605485018	22.26959706535257	-6.31185879131950	c
10.98698130926157	21.79488160680745	-8.86544936115098	c
10.85559305761168	19.11854475292922	-9.29700170593659	c
10.02133644262662	17.93419258593098	-7.00242407429966	c
9.89498002472673	15.13126887783820	-6.58290091395948	c
8.97462654453831	19.47091477859360	-2.41067150308842	c
10.31401414740802	24.74714910319062	-4.90653637692347	c
12.26105446784903	23.65177793699263	-10.61277400517761	c
11.71541335416169	17.74738388426082	-11.64514178751970	c
2.14930377965485	20.64918609710079	-0.85880355711172	c
2.70327338785051	13.91915867591086	10.71930872425360	c
3.15375811338268	11.26910372274417	11.14141300763964	c
1.48869636716060	9.86667377504489	9.51266262423794	c
-0.02079077242971	11.64951347054658	8.12720864719568	c
0.73500225061644	14.14559968830188	8.86378425759085	c
3.75811367271386	16.07505217814348	12.25504603482166	c
4.67786906545931	10.17266801155604	13.28271035538087	c
1.20194895022714	7.02750567706777	9.45193912615314	c

-2.15854351098627	11.02943037106726	6.35119437365377	c
-0.53673713134791	16.56670377041105	8.07166671297952	c
3.31457774128879	9.22626294439152	2.99008767255413	o
9.41313486868079	9.86907290256046	5.27431199845098	c
9.61502894342156	10.68654218785575	7.85843674585309	c
2.04406728685623	8.50285894683501	1.19918125398199	c
9.52672760838946	7.15932267728201	4.39593025874584	c
10.24791646744618	8.98220350539609	10.05290182189275	c
-0.21432641105054	7.37009953929646	-1.36244538182320	mo
-3.30208420612408	5.55044520269895	1.38147274369994	c
-3.12129614779915	3.96491668502434	-0.80630973274231	c
-4.05278222823760	5.36222292198003	-2.94100490195330	c
-4.77192769340345	7.81377767289499	-2.06932946286817	c
-4.34802659545440	7.93304370849140	0.59814350152824	c
2.26761329327058	5.39829939486071	-3.08969071377514	c
3.65161039724433	4.08159221847737	-4.37592741450991	o
5.72248060058578	3.44281181607770	-8.40805395655021	sm
3.02511447286301	9.63108667332250	-10.32684302279572	c
0.62995315432494	10.66568016770454	-15.68122609473954	c
-1.62523134243744	9.93033438999266	-14.34956223415058	c
4.19726339595995	7.73952784534882	-9.77825731034423	o
1.35931696281532	0.69149328486027	-9.29235410616849	c
2.02983061730803	1.73642152183032	-11.69979646682312	c
4.31777864186041	0.53512094847421	-12.54050874744072	c
5.03263763704935	-1.29664496340473	-10.66170217188075	c
3.23241842462489	-1.16176061031478	-8.63062085851259	c
9.69389005852233	4.05511394802846	-5.09401728340966	c
10.35383558231874	1.83225738937965	-6.50719521843848	c
10.87621810277258	2.59347457028615	-9.06963177971236	c
10.48625424524478	5.27769378659070	-9.23746886534829	c
9.76316158784041	6.17657624481067	-6.77647930368822	c
-1.02214233052873	1.24162022202637	-7.83815640112492	c
0.44601430572854	3.54423430755429	-13.21781172351525	c
5.51132759205944	0.88363993985180	-15.10710191457046	c
6.95973545656392	-3.36329073231640	-11.01170155361047	c
3.13350457113668	-2.87216120858858	-6.35143290689237	c
9.26325507353021	4.18193049376614	-2.28502304039473	c
10.81892968902218	-0.73579862680472	-5.36225673884146	c
12.11987642505073	0.99108467584206	-11.07246299021659	c
10.99485221814975	6.89873013954468	-11.52950300218245	c
9.31543263186659	8.88571175851639	-6.05465805042537	c
1.70451844242061	-4.40418950911458	-6.60040328081692	h
4.97656489018467	-3.81202969267627	-5.99431834870995	h
2.60937627884064	-1.83744032983085	-4.59685130405542	h
-1.66374270416549	3.22398491619480	-8.10190177663464	h
-2.60313062871670	-0.00892317656873	-8.46199624739897	h
1.60661846418669	4.81670554790946	-14.41970968951502	h
-0.86666142749230	2.51179460413153	-14.50803605809801	h
-0.73389450490458	4.75636010948639	-11.97678521976809	h
5.37362198901835	2.86855174453345	-15.78831919838692	h
7.54521171138762	0.36062367271371	-15.11712133892555	h
-0.77336735345463	0.93731877726395	-5.77708485007130	h

4.57063836339430	-0.31492935260766	-16.56756558069831 h
8.44936843312906	-2.83660675560224	-12.38834933978011 h
6.03202694643538	-5.10600528037441	-11.75526069339052 h
7.91211463925681	-3.91094246895998	-9.22229390227120 h
2.01352782924822	14.50087833944642	-16.93885103478649 h
-2.28353201642015	16.26630080442016	-14.71250849718299 h
-4.83482979125085	12.25240903683237	-12.77271951097641 h
2.08062713845737	9.38896993146503	-16.43577120685265 h
-2.19702500472704	7.99664258148307	-13.88098840918734 h
-3.25122027921280	19.82392006396025	3.04387148777000 h
-3.58138991267611	22.16341772310670	-1.52379837588259 h
-4.25941155355290	18.54379747029093	-5.12742737382180 h
-4.26344925074182	13.97217443699261	-2.82869795305392 h
-3.66823621268756	14.72855751478762	2.23381680515987 h
-2.82155722620229	4.99951145328016	3.32340668259790 h
-2.46198009708161	1.99759619551036	-0.82819156531254 h
-4.21443494788395	4.66862600172051	-4.88680946089385 h
-5.55757867876956	9.32672621461028	-3.25315453837616 h
-4.78951363890673	9.54011513561381	1.82897329034517 h
3.47238188786657	9.92304870446174	14.99684287285874 h
6.27408206977958	11.41359462047031	13.84389638410373 h
5.47782793321902	8.28677801149004	12.82827841712478 h
2.44993862447961	16.59700538741467	13.82673927539700 h
4.03775692171138	17.81553119741853	11.10901546186286 h
5.60331032640201	15.60201565570437	13.13070010661522 h
0.77391257956731	18.20764731751627	8.10341901276195 h
-2.13670172272779	17.03761572382374	9.36502856402014 h
-1.32465242547905	16.44578216859751	6.13029296959660 h
-1.80928145967207	11.68307063099470	4.38187325038038 h
-3.95994437789433	11.91606035923433	6.98917797155006 h
-2.48718981952801	8.96122419522905	6.24870201535622 h
2.90961516002025	6.05200162448075	10.19045283574373 h
0.86395482831883	6.29520352498225	7.51043099777522 h
-0.41866327866358	6.38810684692070	10.64118600066909 h
9.72087893663448	14.16199147503944	11.93542508155594 h
9.21814310636007	16.91359608200773	10.03223773935624 h
12.28561645303285	15.51635123071425	10.20263073760392 h
9.94365560180705	9.91932980908928	11.90261997366834 h
9.12742369930024	7.20398840616811	10.05921882604274 h
12.27768836528409	8.40984022842229	9.98399295817176 h
8.60387702347643	17.28381196407483	2.63315801460206 h
11.65863747605181	17.50913711369817	4.06612432447369 h
8.90111877258408	18.31901769129565	5.84060004710399 h
7.86259766504186	13.32969584712283	0.01918776784184 h
11.20232040069276	12.79371514918222	0.10615834530114 h
9.05595855723060	10.17957077149385	0.05961758025610 h
8.31079039203780	6.80673882193915	2.72270693463742 h
11.49092079612567	6.60947317427860	3.85746321085828 h
8.91729510946413	5.82326578965436	5.89878240184001 h
10.72461577491173	-2.27720957226667	-6.78276006281157 h
12.73243926002425	-0.84053391847289	-4.47983905335027 h
9.43491948263933	-1.19236554087817	-3.84778507348078 h

7.70514486912596	9.12498796332075	-4.72510174496743	h
11.00952841229098	9.71849873214358	-5.11754827492524	h
8.90024540398074	10.06551261373887	-7.73333620337412	h
11.34402547338949	1.32046018359443	-12.99891808537271	h
14.18420570364853	1.41224803074521	-11.17723667581553	h
11.94043628468094	-1.05651406871620	-10.66463761518487	h
11.11584439597295	5.75006430898170	-13.28389608133489	h
9.51503134716326	8.36110817871670	-11.83664926692350	h
12.82721389256745	7.92818114957753	-11.34898939303041	h
12.00515933363541	19.06302297882818	-13.25496577058281	h
10.34299817700188	16.28096296773941	-12.26899552195993	h
13.55090850136844	16.75835813599918	-11.32397506671932	h
11.60568741886945	23.50066480739500	-12.60534508925958	h
14.34384292251249	23.32030500338117	-10.64012446328401	h
11.97144514761948	25.63514508026147	-10.00609751468871	h
10.23880477946575	26.40190585836734	-6.19504987763848	h
12.11718181547638	24.89957974041155	-3.82166933747946	h
8.75548645072475	24.96744270270965	-3.51487796131260	h
8.48433752184170	14.59154923267303	-5.12500420399657	h
11.76298220015823	14.37406334443227	-5.96223439982498	h
9.38261694094001	14.11982805411773	-8.34804076136548	h
7.86009878738583	21.05125292007549	-1.59641715318605	h
10.74010563811519	19.31016426117795	-1.26724441475237	h
7.87253299032957	17.71022858889054	-2.10376515856264	h
1.48999991054600	19.51862073765509	-14.66116740019189	h
-0.96687638559144	21.83962663519305	-14.49911154073712	h
-0.76086554707417	19.40994653378473	-12.13477093885957	h
5.26745405136165	21.35626190414908	-15.96439271236976	h
4.52494926689040	24.58355989688053	-16.62090306200262	h
7.50785163104983	23.78962432679625	-15.24798253604335	h
-1.86189507769131	21.10437023715478	-8.34573695252407	h
-2.30825979940261	24.46131187384374	-8.15617650169625	h
-0.58070691801558	22.83537651757704	-5.73739462754812	h
1.85013680998352	28.28671926834028	-6.45027458434072	h
5.16614722496296	27.80211158525382	-6.00651408177853	h
2.94176108293108	25.72689254950829	-4.53127282371668	h
8.47080347757187	26.95865722397134	-12.49343112182945	h
8.02624045367683	27.94306505597820	-9.28369202253196	h
6.05568463630069	29.18709790911311	-11.72322801657559	h
8.40854315501570	2.42222037712529	-1.52132168050472	h
11.08139350831705	4.47952837430000	-1.25784748038556	h
7.99097242782069	5.76586760750291	-1.76082823427631	h

[{CpMo(CO)$_2$}$_2$(μ,$\eta^{2:2}$-P$_2$)]

0.09407901850490	2.91489791484149	1.09743837180690	mo
-0.09407901850490	-2.91489791484149	1.09743837180690	mo
1.22544185379829	5.17160795468834	3.86298371796475	c
-1.22544185379829	-5.17160795468834	3.86298371796475	c
3.68984332704307	2.51685562417895	0.16206375272972	c
-3.68984332704307	-2.51685562417895	0.16206375272972	c
1.83521143869115	6.63732163707562	5.39352607806425	o
-1.83521143869115	-6.63732163707562	5.39352607806425	o

5.79697181476800	2.43138898495034	-0.51452909616275	o
-5.79697181476800	-2.43138898495034	-0.51452909616275	o
-2.91221333430228	6.08997395260062	0.29402465023298	c
-4.07483525433803	3.78130365325948	-0.49707393823989	c
-2.63282310796967	2.78370115167377	-2.56809433136993	c
-0.56887739286940	4.46519268262623	-3.04344145108126	c
-0.72896813762676	6.52593385655267	-1.28266027556845	c
-3.59768525219779	7.34489165299907	1.79834979349223	h
-5.79798150371368	2.94190195625628	0.29319482156701	h
-3.08128229182976	1.06870125326766	-3.64033247559632	h
0.85614779244529	4.25692298137993	-4.53798658828945	h
0.52383396620456	8.17803109916201	-1.21547372344437	h
2.91221333430228	-6.08997395260062	0.29402465023298	c
0.72896813762676	-6.52593385655267	-1.28266027556845	c
4.07483525433803	-3.78130365325948	-0.49707393823989	c
0.56887739286940	-4.46519268262623	-3.04344145108126	c
2.63282310796967	-2.78370115167377	-2.56809433136993	c
3.59768525219779	-7.34489165299907	1.79834979349223	h
-0.52383396620456	-8.17803109916201	-1.21547372344437	h
5.79798150371368	-2.94190195625628	0.29319482156701	h
-0.85614779244529	-4.25692298137993	-4.53798658828945	h
3.08128229182976	-1.06870125326766	-3.64033247559632	h
1.99022988687440	-0.23604424194771	4.39801069389469	p
-1.99022988687440	0.23604424194771	4.39801069389469	p

$Na_4P_2^{2+}$

1.94929529295146	0.00000000000000	0.00000000000000	p
-1.94929529295146	0.00000000000000	0.00000000000000	p
4.63910311631087	4.57407968308229	0.00000000000000	na
-4.63910311631087	-4.57407968308229	0.00000000000000	na
4.63910311631087	-4.57407968308229	0.00000000000000	na
-4.63910311631087	4.57407968308229	0.00000000000000	na

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