ESI

Light induced dissolution and concomitant crystallization of a Keggin-type polyoxometalate mimicking a Naturally occurring phenomenon

S1 Fourier Transform Infrared (FTIR) Spectroscopic Analysis

The infrared spectra for the polycrystalline parent compound is shown in **Figure S2**.

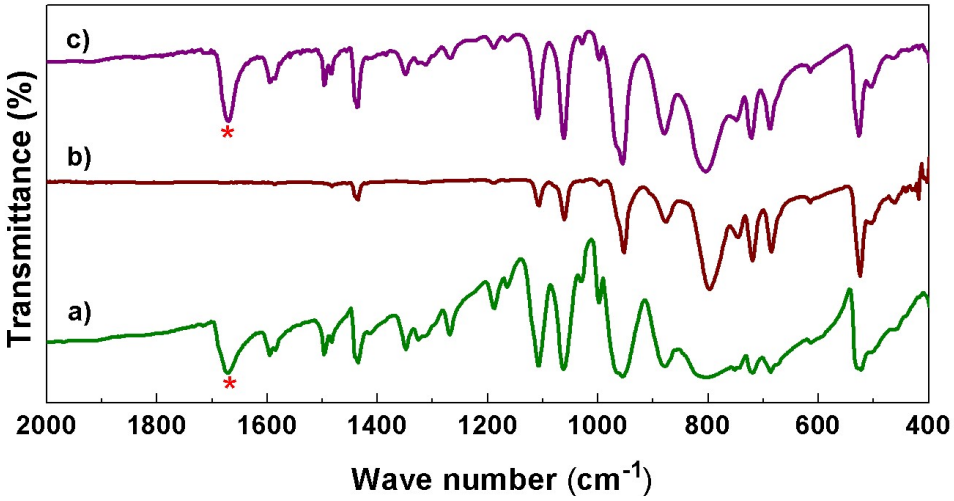


Fig. S1. Comparative IR spectra for a) Compound **1**; b) Compound **2**; c) Compound **3**. The marked peaks represent the carbonyl stretching of the NMF solvent.

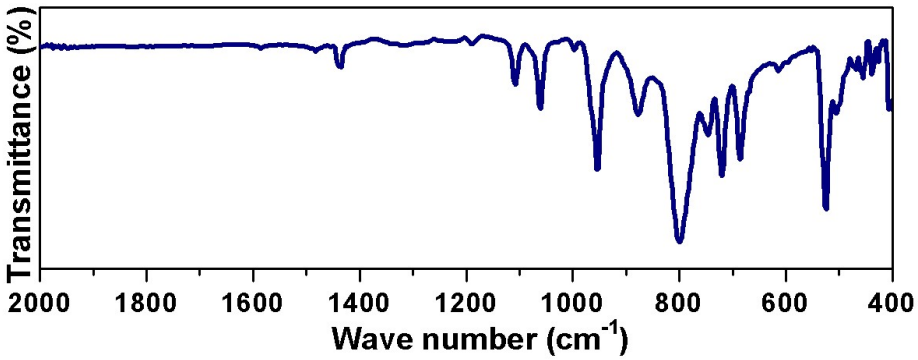


Fig. S2. Infrared spectra for compound polycrystalline parent

IR bands for Compound polycrystalline parent compound: $\bar{\upsilon}$ = 1435 (s, ν(C=C)), 1104 (s, ν_s(P-C)), 1060 (m, $\nu_{as}(PO_4)$), 952 (m, ν(Mo=O_t)), 879 (s), 794 (s), 714 (m), 680 (s, ν(C-H)), 522 (s), 408 (s) cm^{-1}.

S2 Powder X-Ray Diffraction (PXRD) Analysis

The powder XRD pattern for the polycrystalline parent compound is shown in **Figure S3**

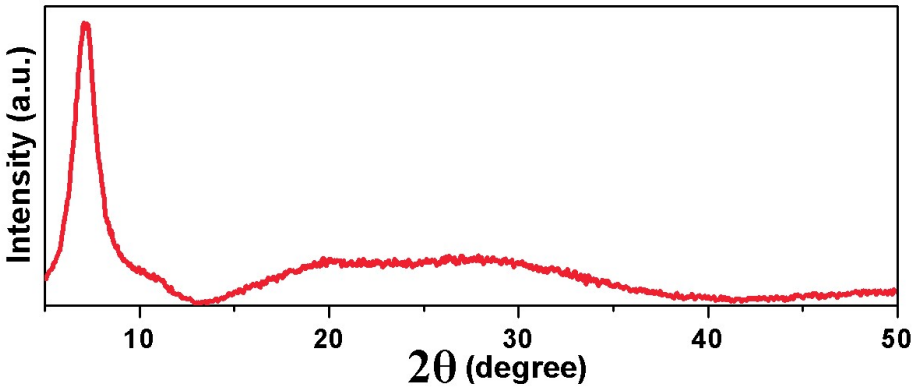


Fig. S3. Powder X-ray pattern for parent compound

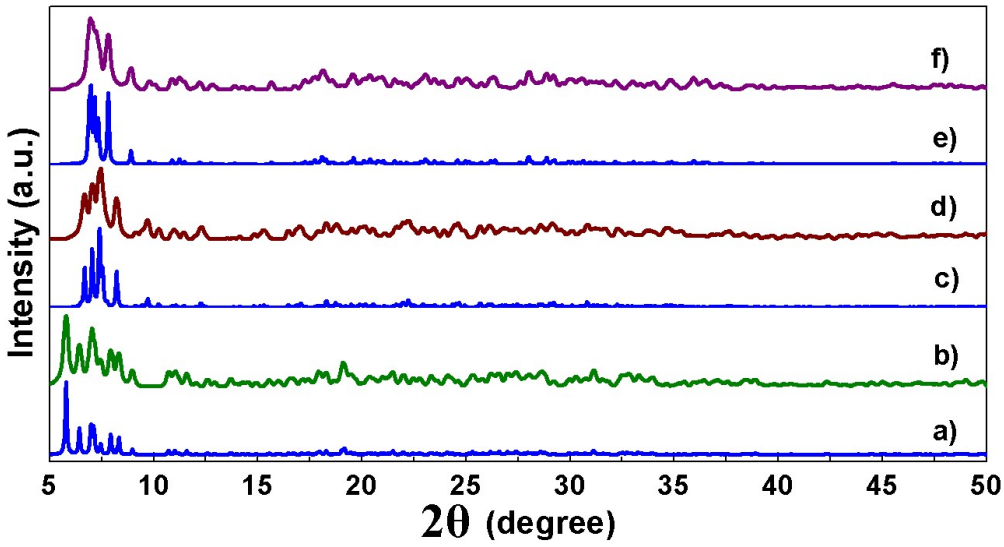


Fig. S4. a) Simulated powder XRD pattern for compound **1**; b) Powder XRD pattern for as synthesized compound **1**; c) Simulated powder XRD pattern for compound **2**; d) Powder XRD pattern for as synthesized **2**; e) Simulated powder pattern for compound **3**; f) Powder XRD pattern for as synthesized compound **3**.

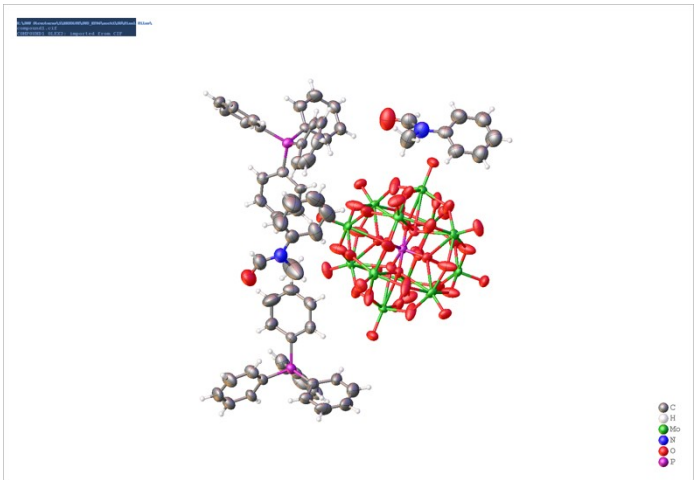
S3 Single Crystal X-ray Crystallography

compound1

Olex2
Report created with ReportPlus

R_1=6.80%

Crystal Data and Experimental



Experimental. Single clear dark green block-shaped crystals of **compound1** recrystallised from N-Methyl Formanilide by slow evaporation. A suitable crystal with dimensions 0.22 × 0.20 × 0.19 mm^3 was selected and mounted on a Bruker APEX-II CCD diffractometer. The crystal was kept at a steady T = 292(2) K during data collection. The structure was solved with the ShelXT 2018/2 (Sheldrick, 2018) solution program using iterative methods and by using Olex2 1.5-alpha (Dolomanov et al., 2009) as the graphical interface. The model was refined with ShelXL 2018/3 (Sheldrick, 2015) using full matrix least squares minimisation on F^2.

Crystal Data. $C_{120}H_{107}Mo_{12}N_3O_{43}P_5$, M_r = 3585.21, triclinic, P-1 (No. 2), a = 14.9244(8) Å, b = 14.9531(9) Å, c = 16.6482(9) Å, α = 84.920(3)°, β = 66.901(2)°, γ = 67.164(2)°, V = 3140.7(3) Å^3, T = 292(2) K, Z = 1, Z' = 0.5, μ(MoK$_\alpha$) = 1.304, 90355 reflections measured, 10960 unique (R_{int} = 0.0363) which were used in all calculations. The final wR_2 was 0.1442 (all data) and R_1 was 0.0680 (I≥2 σ(I)).

Compound	**compound1**
Formula	$C_{120}H_{107}Mo_{12}N_3O_{43}P_5$
$D_{calc.}$/ g cm^{-3}	1.896
μ/mm^{-1}	1.304
Formula Weight	3585.21
Colour	clear dark green
Shape	block-shaped
Size/mm^3	0.22×0.20×0.19
T/K	292(2)
Crystal System	triclinic
Space Group	P-1
a/Å	14.9244(8)
b/Å	14.9531(9)
c/Å	16.6482(9)
α/°	84.920(3)
β/°	66.901(2)
γ/°	67.164(2)
V/Å^3	3140.7(3)
Z	1
Z'	0.5
Wavelength/Å	0.71073
Radiation type	MoK$_\alpha$
Θ_{min}/°	2.457
Θ_{max}/°	24.999
Measured Refl's.	90355
Indep't Refl's	10960
Refl's I≥2 σ(I)	9992
R_{int}	0.0363
Parameters	868
Restraints	526
Largest Peak	0.826
Deepest Hole	-0.985
GooF	1.362
wR_2 (all data)	0.1442
wR_2	0.1419
R_1 (all data)	0.0741
R_1	0.0680

Structure Quality Indicators

Reflections:	d min (Mo) 2Θ=50.0° 0.84	I/σ(I) CIF 46.9	Rint CIF 3.63%	Full 50.0° 99.0
Refinement:	Shift CIF 0.001	Max Peak CIF 0.8	Min Peak CIF -1.0	GooF CIF 1.362

A clear dark green block-shaped-shaped crystal with dimensions 0.22 × 0.20 × 0.19 mm^3 was mounted. Data were collected using a Bruker APEX-II CCD diffractometer operating at T = 292(2) K.

Data were measured using ϕ and ω scans with MoK_α radiation. . The maximum resolution that was achieved was Θ = 24.999° (0.84 Å).

The unit cell was refined using SAINT v8.34A (Bruker, 2013) on 9990 reflections, 11% of the observed reflections.

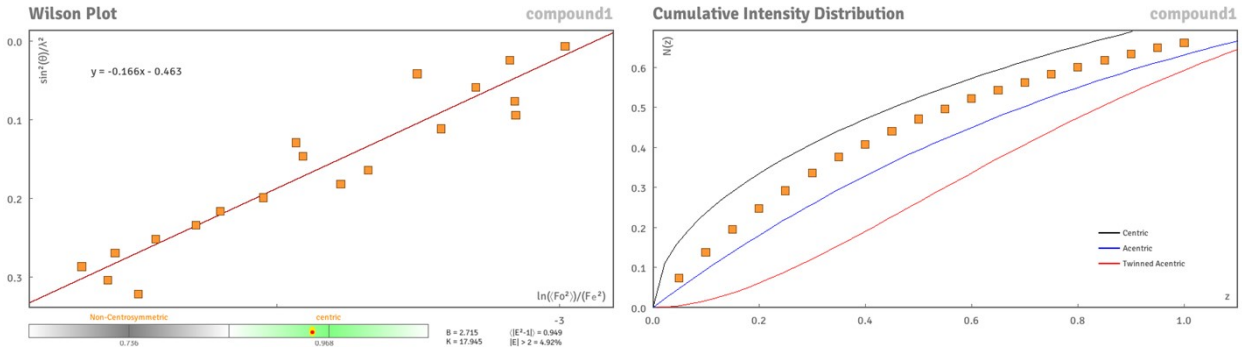
Data reduction, scaling and absorption corrections were performed using SAINT v8.34A (Bruker, 2013). The final completeness is 99.00 % out to 24.999° in Θ. SADABS-2008/1 (Bruker, 2008) was used for absorption correction. wR_2(int) was 0.0725 before and 0.0497 after correction. The Ratio of minimum to maximum transmission is 0.6868. The $\lambda/2$ correction factor is 0.0015. The absorption coefficient μ of this material is 1.304 mm^{-1} at this wavelength (λ = 0.71073Å) and the minimum and maximum transmissions are 0.066 and 0.096.

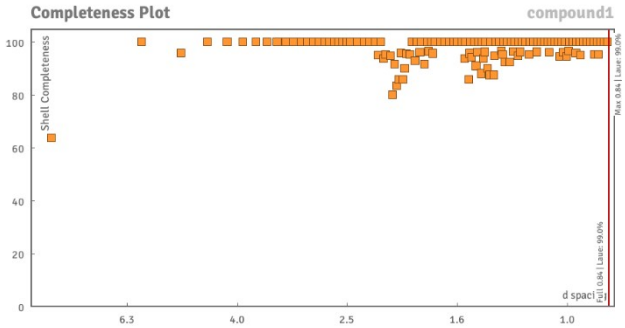
The structure was solved and the space group P-1 (# 2) determined by the ShelXT 2018/2 (Sheldrick, 2018) structure solution program using using iterative methods and refined by full matrix least squares minimisation on $\boldsymbol{F^2}$ using version 2018/3 of ShelXL 2018/3 (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model.

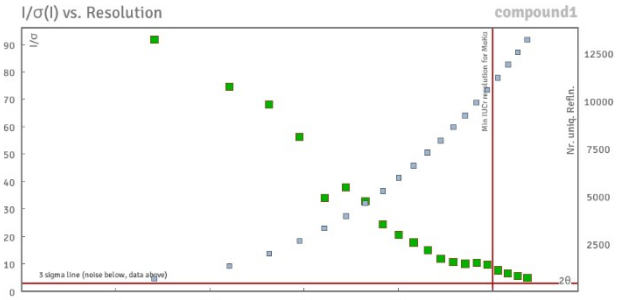
_exptl_absorpt_process_details: SADABS-2008/1 (Bruker,2008) was used for absorption correction.wR_2(int) was 0.0725 before and 0.0497 after correction.The Ratio of minimum to maximum transmission is 0.6868.The $\lambda/2$ correction factor is 0.0015.

The value of Z' is 0.5. This means that only half of the formula unit is present in the asymmetric unit, with the other half consisting of symmetry equivalent atoms. The moiety formula is Mo12 O40 P, 4(C24 H20 P), 3(C8 H9 N O).

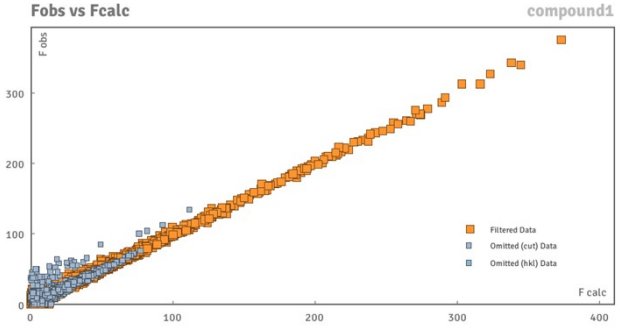
Data Plots: Diffraction Data

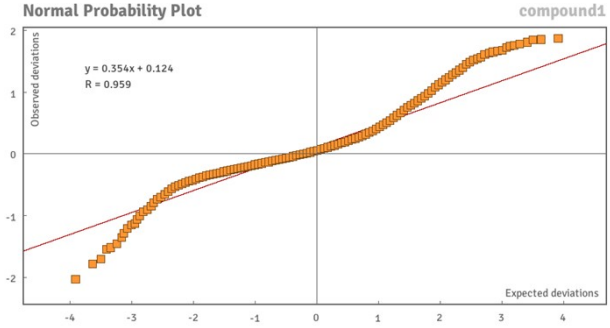






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	91400	Unique reflections	10960
Completeness	0.991	Mean I/σ	32.77
hkl_{max} collected	(19, 19, 21)	hkl_{min} collected	(-19, -19, -21)
hkl_{max} used	(17, 17, 19)	hkl_{min} used	(-15, -17, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.84
d_{max} used	8.29	d_{min} used	0.84
Friedel pairs	13846	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0363
R_{sigma}	0.0213	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	1045
Multiplicity	(934, 6346, 6875, 5192, 3563, 2530, 1356, 478, 249, 149, 28)	Maximum multiplicity	18
Removed systematic absences	0	Filtered off (Shel/OMIT)	13969

There are no images if the crystal on the diffractometer, but the inclusion of these images has been requested from the GUI. Please unitck the relevant box if you don't have these images!

Table 1: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **compound1**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Mo6	1305.5(7)	7475.8(5)	4324.8(5)	34.8(2)
Mo1	1413.0(6)	11543.7(6)	4280.8(5)	33.7(2)
Mo5	-591.5(6)	9029.1(6)	3487.3(5)	34.8(2)
Mo3	1045.9(6)	10381.6(6)	2726.5(5)	35.7(2)
Mo4	-1711.5(6)	11579.5(6)	4011.9(6)	36.8(2)
Mo2	2775.4(6)	8990.1(6)	3770.0(5)	36.4(2)
P1	0	10000	5000	29.3(7)
P3	6580(2)	6818.9(18)	4728.6(17)	37.7(6)
P2	1405(2)	5490.5(19)	675.0(17)	40.9(6)

Atom	x	y	z	U_{eq}
O20	-2536(5)	12290(5)	3557(5)	47.6(17)
O18	4067(5)	8482(5)	3176(5)	51.1(18)
O13	-1372(5)	8680(6)	4546(5)	61(2)
O11	635(6)	7937(6)	3568(5)	62(2)
O22	1909(6)	6280(5)	4036(5)	60(2)
O19	1518(6)	10602(5)	1673(4)	53.4(18)
O14	2374(7)	7908(7)	3713(5)	69(2)
O7	2226(6)	9446(5)	2849(5)	57.3(19)
O16	1621(7)	7533(7)	5361(5)	71(2)
O12	-34(6)	7557(6)	5226(5)	64(2)
O6	2563(7)	10260(5)	3991(6)	69(2)
O21	-800(6)	8517(6)	2767(5)	53.5(18)
O8	-415(6)	11356(5)	3116(7)	75(3)
O5	1257(7)	11331(5)	3266(5)	67(2)
O15	2714(7)	8655(7)	4890(5)	67(2)
O10	491(6)	9467(5)	2703(6)	67(2)
O9	-1548(6)	10293(5)	3657(6)	72(2)
O17	2094(6)	12259(6)	3952(6)	67(2)
C43	7991(7)	6184(7)	4338(6)	38(2)
C31	6311(8)	8014(7)	4373(7)	41(2)
C44	8634(8)	6644(7)	3812(6)	42(2)
C37	6011(8)	6853(7)	5906(6)	40(2)
C26	4984(8)	6689(7)	4364(6)	42(2)
C45	9724(8)	6182(7)	3524(7)	47(2)
C30	6506(8)	5233(7)	4037(7)	47(2)
C19	2155(8)	5873(7)	1096(6)	42(2)
C25	6016(8)	6212(7)	4316(6)	41(2)
C27	4485(9)	6209(8)	4135(7)	52(3)
C7	2310(8)	4766(7)	-320(6)	44(2)
C36	6175(10)	8235(9)	3583(8)	61(3)
N1	5249(9)	8417(8)	405(8)	74(3)
C13	423(9)	6538(7)	475(7)	49(3)
C23	2365(10)	7086(9)	1772(8)	60(3)
C32	6379(7)	8715(7)	4824(8)	46(2)
C1	799(9)	4760(7)	1418(6)	47(2)
C28	5009(9)	5245(9)	3853(7)	54(3)
C33	6339(8)	9592(8)	4485(9)	59(3)
C34	6220(10)	9788(8)	3710(10)	70(4)
C8	2245(9)	3924(8)	-543(7)	53(3)
C24	1781(9)	6807(8)	1451(7)	52(3)
C48	8427(9)	5259(7)	4587(7)	50(3)
C6	1447(11)	3942(9)	1684(8)	64(3)
C14	-414(9)	7161(8)	1169(9)	62(3)
C46	10158(9)	5252(8)	3771(8)	55(3)
C4	-32(15)	3519(12)	2499(9)	88(5)
C42	4915(9)	7192(8)	6334(7)	54(3)
O23	5909(9)	7171(8)	-593(8)	105(4)
C22	3316(11)	6419(9)	1757(9)	67(3)
O4	1022(10)	9084(9)	4819(8)	39(2)
C15	-1127(11)	7999(9)	993(11)	76(4)
C5	1027(14)	3337(10)	2223(9)	80(4)
C41	4445(10)	7204(9)	7225(8)	65(3)
C20	3144(10)	5206(9)	1042(9)	65(3)
C47	9507(9)	4791(8)	4281(8)	57(3)
C38	6615(9)	6559(9)	6400(8)	57(3)
C2	-259(9)	4930(8)	1673(7)	56(3)
C29	5999(10)	4766(7)	3801(7)	54(3)
C40	5065(10)	6895(9)	7699(8)	66(3)
C10	3784(11)	3629(11)	-1850(9)	78(4)
C18	540(10)	6766(8)	-378(8)	59(3)
C3	-673(12)	4314(11)	2249(9)	77(4)
C11	3822(12)	4496(11)	-1671(8)	79(4)
C39	6124(11)	6584(11)	7296(8)	73(4)

Atom	x	y	z	U_{eq}
C16	-1012(11)	8213(9)	164(11)	79(4)
C12	3104(10)	5055(10)	-901(7)	64(3)
C9	2986(11)	3369(9)	-1315(8)	67(3)
C35	6124(12)	9118(11)	3266(11)	88(5)
C52	5518(11)	10681(7)	1482(8)	110(5)
C51	6355(8)	10109(9)	753(9)	142(8)
C50	6270(7)	9362(8)	386(6)	117(6)
C49	5347(8)	9186(6)	748(6)	66(3)
C54	4509(7)	9758(7)	1478(6)	88(4)
C53	4595(9)	10505(7)	1845(6)	107(5)
C17	-198(13)	7604(10)	-529(11)	82(4)
C56	5945(13)	7872(10)	-283(10)	84(4)
C21	3737(13)	5495(13)	1361(13)	104(6)
C55	4290(18)	8210(20)	841(15)	185(12)
O2	-221(9)	10153(8)	4136(8)	36(2)
O3	-118(10)	9120(8)	4766(8)	35(2)
O24	2520(20)	7734(17)	9245(16)	118(8)
C58	-83(15)	10019(17)	10774(12)	88(8)
C57	211(12)	9882(16)	9878(12)	63(4)
C62	-489(16)	10413(16)	9491(9)	75(6)
C61	-1483(14)	11082(15)	10000(15)	98(10)
C60	-1777(13)	11219(16)	10897(14)	101(10)
C59	-1077(17)	10687(17)	11284(9)	90(8)
O1	927(10)	10177(9)	4269(8)	38(2)
C63	1680(30)	9280(30)	8458(19)	102(12)
C64	1680(30)	8420(20)	9640(20)	81(8)
N2	1188(15)	9227(16)	9347(14)	79(6)

Table 2: Anisotropic Displacement Parameters ($\times 10^4$) for **compound1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mo6	43.2(5)	19.9(4)	39.0(5)	1.9(3)	-17.6(4)	-8.3(3)
Mo1	37.3(4)	30.2(4)	41.6(5)	10.7(3)	-17.5(4)	-20.7(3)
Mo5	36.6(4)	33.1(4)	39.3(5)	-4.3(3)	-17.2(4)	-14.0(3)
Mo3	38.2(5)	32.4(4)	26.4(4)	7.9(3)	-6.7(3)	-10.7(4)
Mo4	33.1(4)	33.9(4)	48.5(5)	17.1(4)	-24.4(4)	-12.4(3)
Mo2	23.2(4)	44.9(5)	33.7(4)	1.5(4)	-7.6(3)	-8.9(3)
P1	29.3(16)	26.9(16)	32.2(17)	6.0(13)	-13.5(13)	-10.7(13)
P3	39.8(13)	33.4(13)	45.6(14)	10.9(11)	-21.5(12)	-16.8(11)
P2	47.1(15)	36.4(13)	38.2(14)	1.7(11)	-19.2(12)	-12.4(11)
O20	49(4)	46(4)	59(4)	17(3)	-36(4)	-17(3)
O18	32(4)	59(4)	51(4)	-6(3)	-13(3)	-8(3)
O13	37(4)	86(6)	45(4)	19(4)	-18(3)	-9(4)
O11	43(4)	82(5)	40(4)	11(4)	-17(3)	-4(4)
O22	80(5)	25(3)	47(4)	5(3)	-8(4)	-9(3)
O19	69(5)	47(4)	38(4)	11(3)	-18(3)	-21(4)
O14	99(6)	104(6)	41(4)	17(4)	-31(4)	-76(5)
O7	71(5)	37(4)	65(4)	-6(3)	-48(4)	2(3)
O16	112(7)	112(7)	45(4)	36(4)	-44(5)	-92(6)
O12	47(4)	81(5)	46(4)	23(4)	-18(3)	-12(4)
O6	88(6)	43(4)	83(6)	-3(4)	-65(5)	0(4)
O21	51(4)	70(5)	43(4)	-12(4)	-18(3)	-24(4)
O8	41(4)	25(4)	129(7)	1(4)	-2(4)	-11(3)
O5	100(6)	30(4)	79(5)	0(3)	-68(5)	-1(4)
O15	99(6)	106(7)	44(4)	28(4)	-37(4)	-83(6)
O10	38(4)	35(4)	100(6)	-6(4)	2(4)	-14(3)
O9	39(4)	35(4)	120(7)	-1(4)	-4(4)	-17(3)
O17	70(5)	68(5)	96(6)	42(5)	-51(5)	-49(5)
C43	40(5)	37(5)	42(5)	10(4)	-23(4)	-13(4)
C31	42(5)	35(5)	48(6)	11(4)	-22(5)	-14(4)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C44	55(6)	42(5)	41(5)	8(4)	-19(5)	-29(5)
C37	52(6)	36(5)	44(6)	6(4)	-24(5)	-24(5)
C26	46(6)	46(6)	43(6)	10(4)	-27(5)	-19(5)
C45	41(6)	45(6)	52(6)	2(5)	-15(5)	-16(5)
C30	50(6)	40(6)	48(6)	10(5)	-18(5)	-17(5)
C19	51(6)	41(5)	37(5)	2(4)	-17(5)	-20(5)
C25	45(6)	39(5)	48(6)	11(4)	-19(5)	-27(5)
C27	45(6)	55(7)	61(7)	6(5)	-26(5)	-19(5)
C7	48(6)	42(6)	38(5)	-2(4)	-20(5)	-10(5)
C36	79(9)	59(7)	55(7)	23(6)	-35(6)	-32(7)
N1	72(6)	68(5)	77(6)	-2(4)	-30(5)	-19(4)
C13	57(7)	36(5)	61(7)	4(5)	-33(6)	-16(5)
C23	67(8)	58(7)	55(7)	-6(6)	-12(6)	-34(6)
C32	33(5)	33(5)	70(7)	6(5)	-23(5)	-10(4)
C1	61(7)	43(6)	36(5)	3(4)	-18(5)	-21(5)
C28	68(8)	64(7)	53(7)	13(6)	-34(6)	-39(6)
C33	43(6)	38(6)	93(10)	-4(6)	-27(6)	-11(5)
C34	64(8)	34(6)	103(11)	24(7)	-27(8)	-20(6)
C8	63(7)	48(6)	43(6)	-10(5)	-21(5)	-13(5)
C24	46(6)	51(6)	51(6)	0(5)	-12(5)	-15(5)
C48	55(7)	41(6)	64(7)	26(5)	-35(6)	-21(5)
C6	74(8)	53(7)	55(7)	8(6)	-17(6)	-24(6)
C14	48(7)	55(7)	80(9)	-17(6)	-26(6)	-9(6)
C46	46(6)	53(7)	65(7)	-1(6)	-30(6)	-9(5)
C4	132(15)	76(10)	65(9)	7(8)	-14(10)	-74(11)
C42	49(6)	64(7)	44(6)	-8(5)	-18(5)	-13(6)
O23	117(9)	72(6)	121(9)	-20(5)	-56(7)	-15(6)
C22	89(10)	61(8)	81(9)	15(7)	-53(8)	-41(8)
O4	41(5)	31(5)	45(7)	8(5)	-24(5)	-9(4)
C15	73(9)	50(8)	100(11)	-8(7)	-41(8)	-7(7)
C5	115(13)	52(8)	59(8)	12(6)	-23(8)	-30(8)
C41	54(7)	74(9)	59(8)	-13(6)	-14(6)	-21(6)
C20	60(7)	47(7)	91(10)	-3(6)	-40(7)	-11(6)
C47	63(7)	37(6)	79(8)	12(6)	-45(7)	-11(5)
C38	55(7)	71(8)	54(7)	11(6)	-24(6)	-31(6)
C2	57(7)	54(7)	53(7)	-2(5)	-11(6)	-26(6)
C29	71(8)	32(5)	62(7)	-2(5)	-27(6)	-20(5)
C40	68(8)	74(9)	53(7)	-6(6)	-17(6)	-29(7)
C10	64(8)	95(11)	54(8)	-28(7)	-9(7)	-15(8)
C18	72(8)	46(6)	71(8)	9(6)	-45(7)	-18(6)
C3	87(10)	85(10)	61(8)	-8(7)	-7(7)	-56(9)
C11	88(10)	103(11)	42(7)	-6(7)	-11(7)	-45(9)
C39	84(10)	95(10)	54(8)	19(7)	-42(7)	-35(8)
C16	78(9)	43(7)	120(13)	-9(8)	-64(10)	2(7)
C12	77(9)	73(8)	47(7)	3(6)	-18(6)	-40(7)
C9	79(9)	62(8)	59(8)	-15(6)	-27(7)	-22(7)
C35	91(11)	89(11)	102(12)	55(10)	-60(10)	-39(9)
C52	168(12)	72(9)	115(11)	13(7)	-92(9)	-35(8)
C51	150(12)	122(12)	169(13)	-24(10)	-55(10)	-67(9)
C50	90(7)	105(11)	143(12)	-32(9)	-19(7)	-43(8)
C49	74(6)	60(5)	62(6)	8(4)	-36(4)	-15(4)
C54	110(8)	64(7)	66(6)	4(5)	-21(5)	-22(6)
C53	156(11)	67(8)	90(9)	2(6)	-61(8)	-21(8)
C17	112(12)	63(9)	104(12)	24(8)	-85(11)	-26(9)
C56	88(8)	67(6)	85(7)	-9(5)	-30(5)	-17(6)
C21	88(11)	107(13)	148(17)	13(12)	-77(12)	-39(10)
C55	152(12)	250(30)	149(17)	-79(17)	22(12)	-141(17)
O2	34(6)	25(5)	42(5)	3(4)	-15(5)	-4(5)
O3	42(6)	24(5)	44(6)	4(4)	-16(5)	-19(5)
O24	110(14)	94(13)	104(15)	27(11)	-20(12)	-19(9)
C58	94(14)	110(20)	67(9)	8(9)	-33(8)	-41(12)
C57	73(10)	71(10)	66(8)	14(8)	-30(7)	-46(7)
C62	75(10)	87(15)	75(11)	20(11)	-34(9)	-41(9)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C61	83(11)	110(20)	90(12)	13(13)	-28(10)	-31(11)
C60	87(15)	120(20)	90(12)	11(13)	-25(11)	-43(14)
C59	92(14)	101(19)	82(12)	2(12)	-28(9)	-49(12)
O1	37(6)	35(6)	37(6)	0(4)	-4(4)	-18(5)
C63	84(18)	120(30)	68(10)	31(10)	-23(9)	-17(17)
C64	93(14)	83(12)	67(13)	21(10)	-36(10)	-32(9)
N2	81(10)	84(11)	67(9)	24(8)	-26(8)	-33(8)

Table 3: Bond Lengths in Å for **compound1**.

Atom	Atom	Length/Å
Mo6	O11	1.834(7)
Mo6	O22	1.674(7)
Mo6	O14	1.845(8)
Mo6	O16	1.975(7)
Mo6	O12	1.936(7)
Mo6	O4	2.435(12)
Mo6	O3	2.478(12)
Mo1	$O13^1$	1.932(7)
Mo1	$O12^1$	1.855(8)
Mo1	O6	1.955(7)
Mo1	O5	1.863(7)
Mo1	O17	1.668(7)
Mo1	$O3^1$	2.458(12)
Mo1	O1	2.424(12)
Mo5	O13	1.853(7)
Mo5	O11	1.967(7)
Mo5	O21	1.663(7)
Mo5	O10	1.938(7)
Mo5	O9	1.836(7)
Mo5	O2	2.409(12)
Mo5	O3	2.521(12)
Mo3	O19	1.671(7)
Mo3	O7	1.849(7)
Mo3	O8	1.972(7)
Mo3	O5	1.928(7)
Mo3	O10	1.864(7)
Mo3	O2	2.466(12)
Mo3	O1	2.503(13)
Mo4	O20	1.671(6)
Mo4	$O16^1$	1.834(8)
Mo4	O8	1.845(8)
Mo4	$O15^1$	1.962(7)
Mo4	O9	1.958(8)
Mo4	$O4^1$	2.504(12)
Mo4	O2	2.478(11)
Mo2	O18	1.664(7)
Mo2	O14	1.953(8)
Mo2	O7	1.964(7)
Mo2	O6	1.845(8)
Mo2	O15	1.863(7)
Mo2	O4	2.467(13)
Mo2	O1	2.473(12)
P1	O4	1.544(12)
P1	$O4^1$	1.544(12)
P1	O2	1.577(12)
P1	$O2^1$	1.577(12)
P1	O3	1.497(11)
P1	$O3^1$	1.497(11)
P1	O1	1.539(12)
P1	$O1^1$	1.539(12)
P3	C43	1.802(10)
P3	C31	1.774(9)
P3	C37	1.801(10)
P3	C25	1.777(9)
P2	C19	1.805(10)
P2	C7	1.780(10)
P2	C13	1.794(10)
P2	C1	1.786(11)
C43	C44	1.380(13)
C43	C48	1.386(13)
C31	C36	1.400(14)
C31	C32	1.399(14)
C44	C45	1.389(14)
C37	C42	1.396(14)
C37	C38	1.375(14)
C26	C25	1.396(13)
C26	C27	1.379(14)
C45	C46	1.390(15)
C30	C25	1.385(14)
C30	C29	1.380(15)
C19	C24	1.375(14)
C19	C20	1.397(15)
C27	C28	1.367(15)
C7	C8	1.392(14)
C7	C12	1.397(15)
C36	C35	1.362(17)
N1	C49	1.408(13)
N1	C56	1.277(17)
N1	C55	1.47(2)
C13	C14	1.385(15)
C13	C18	1.390(15)
C23	C24	1.381(16)
C23	C22	1.374(17)
C32	C33	1.369(15)
C1	C6	1.396(15)
C1	C2	1.385(15)
C28	C29	1.338(16)
C33	C34	1.360(18)
C34	C35	1.38(2)
C8	C9	1.387(15)
C48	C47	1.375(15)
C6	C5	1.368(17)
C14	C15	1.390(17)
C46	C47	1.381(16)
C4	C5	1.38(2)
C4	C3	1.36(2)
C42	C41	1.368(16)
O23	C56	1.236(17)
C22	C21	1.38(2)
C15	C16	1.35(2)
C41	C40	1.367(17)
C20	C21	1.399(18)

Atom	Atom	Length/Å
C38	C39	1.376(16)
C2	C3	1.405(17)
C40	C39	1.347(18)
C10	C11	1.383(19)
C10	C9	1.352(18)
C18	C17	1.392(16)
C11	C12	1.381(17)
C16	C17	1.37(2)
C52	C51	1.3900
C52	C53	1.3900
C51	C50	1.3900
C50	C49	1.3900
C49	C54	1.3900
C54	C53	1.3900
O24	C64	1.24(4)
C58	C57	1.3900
C58	C59	1.3900
C57	C62	1.3900
C57	N2	1.378(17)
C62	C61	1.3900
C61	C60	1.3900
C60	C59	1.3900
C63	N2	1.38(3)
C64	N2	1.31(3)

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

Table 4: Bond Angles in ° for **compound1**.

Atom	Atom	Atom	Angle/°
O11	Mo6	O14	93.6(4)
O11	Mo6	O16	155.9(4)
O11	Mo6	O12	88.6(3)
O11	Mo6	O4	94.3(4)
O11	Mo6	O3	65.2(4)
O22	Mo6	O11	102.8(4)
O22	Mo6	O14	101.9(4)
O22	Mo6	O16	100.7(4)
O22	Mo6	O12	101.5(4)
O22	Mo6	O4	159.0(4)
O22	Mo6	O3	159.7(4)
O14	Mo6	O16	86.8(3)
O14	Mo6	O12	155.4(4)
O14	Mo6	O4	64.5(4)
O14	Mo6	O3	95.4(4)
O16	Mo6	O4	64.2(4)
O16	Mo6	O3	90.8(4)
O12	Mo6	O16	81.5(3)
O12	Mo6	O4	91.0(4)
O12	Mo6	O3	63.4(4)
O4	Mo6	O3	40.9(4)
O13[1]	Mo1	O6	83.5(3)
O13[1]	Mo1	O3[1]	63.9(4)
O13[1]	Mo1	O1	90.9(4)
O12[1]	Mo1	O13[1]	88.0(3)
O12[1]	Mo1	O6	156.9(4)
O12[1]	Mo1	O5	92.3(4)
O12[1]	Mo1	O3[1]	64.8(4)
O12[1]	Mo1	O1	94.9(4)
O6	Mo1	O3[1]	92.3(4)
O6	Mo1	O1	63.9(4)
O5	Mo1	O13[1]	155.8(4)
O5	Mo1	O6	86.9(3)
O5	Mo1	O3[1]	94.4(4)
O5	Mo1	O1	64.9(4)
O17	Mo1	O13[1]	101.7(4)
O17	Mo1	O12[1]	102.1(4)
O17	Mo1	O6	100.6(4)
O17	Mo1	O5	101.9(4)
O17	Mo1	O3[1]	159.6(4)
O17	Mo1	O1	159.1(4)
O1	Mo1	O3[1]	41.1(4)
O13	Mo5	O11	85.8(3)
O13	Mo5	O10	155.6(4)
O13	Mo5	O2	94.9(4)
O13	Mo5	O3	63.4(4)
O11	Mo5	O2	90.9(4)
O11	Mo5	O3	62.8(4)
O21	Mo5	O13	102.7(4)
O21	Mo5	O11	99.5(4)
O21	Mo5	O10	100.3(4)
O21	Mo5	O9	103.8(4)
O21	Mo5	O2	160.1(4)
O21	Mo5	O3	156.9(4)
O10	Mo5	O11	82.5(3)
O10	Mo5	O2	64.0(4)
O10	Mo5	O3	92.3(4)
O9	Mo5	O13	93.8(4)
O9	Mo5	O11	156.2(4)
O9	Mo5	O10	88.5(3)
O9	Mo5	O2	65.4(4)
O9	Mo5	O3	95.7(4)
O2	Mo5	O3	42.2(4)
O19	Mo3	O7	102.5(4)
O19	Mo3	O8	100.5(4)
O19	Mo3	O5	101.1(4)
O19	Mo3	O10	102.5(4)
O19	Mo3	O2	158.3(4)
O19	Mo3	O1	158.2(4)
O7	Mo3	O8	156.6(4)
O7	Mo3	O5	88.2(3)
O7	Mo3	O10	92.5(3)
O7	Mo3	O2	95.1(4)
O7	Mo3	O1	64.9(4)
O8	Mo3	O2	63.6(4)
O8	Mo3	O1	91.9(4)
O5	Mo3	O8	83.2(4)
O5	Mo3	O2	92.0(4)
O5	Mo3	O1	62.4(4)
O10	Mo3	O8	86.6(3)
O10	Mo3	O5	155.6(4)
O10	Mo3	O2	63.7(4)
O10	Mo3	O1	96.0(4)
O2	Mo3	O1	43.1(4)
O20	Mo4	O16[1]	102.4(4)
O20	Mo4	O8	101.6(4)
O20	Mo4	O15[1]	100.7(4)
O20	Mo4	O9	100.4(4)
O20	Mo4	O4[1]	158.5(4)
O20	Mo4	O2	157.4(4)

Atom	Atom	Atom	Angle/°
O16[1]	Mo4	O8	94.3(4)
O16[1]	Mo4	O15[1]	88.1(3)
O16[1]	Mo4	O9	156.4(4)
O16[1]	Mo4	O4[1]	64.3(4)
O16[1]	Mo4	O2	96.7(4)
O8	Mo4	O15[1]	156.5(4)
O8	Mo4	O9	86.8(3)
O8	Mo4	O4[1]	96.4(4)
O8	Mo4	O2	64.8(4)
O15[1]	Mo4	O4[1]	63.7(4)
O15[1]	Mo4	O2	91.7(4)
O9	Mo4	O15[1]	81.9(3)
O9	Mo4	O4[1]	92.1(4)
O9	Mo4	O2	62.4(4)
O2	Mo4	O4[1]	43.6(4)
O18	Mo2	O14	99.8(4)
O18	Mo2	O7	101.1(3)
O18	Mo2	O6	103.1(4)
O18	Mo2	O15	101.6(4)
O18	Mo2	O4	157.5(4)
O18	Mo2	O1	159.7(4)
O14	Mo2	O7	82.6(3)
O14	Mo2	O4	62.5(4)
O14	Mo2	O1	92.4(4)
O7	Mo2	O4	90.9(4)
O7	Mo2	O1	64.3(4)
O6	Mo2	O14	156.5(4)
O6	Mo2	O7	87.8(3)
O6	Mo2	O15	93.2(4)
O6	Mo2	O4	96.4(4)
O6	Mo2	O1	64.1(4)
O15	Mo2	O14	87.4(3)
O15	Mo2	O7	156.4(4)
O15	Mo2	O4	65.6(4)
O15	Mo2	O1	95.0(4)
O4	Mo2	O1	42.3(4)
O4[1]	P1	O4	180.0
O4	P1	O2	107.3(6)
O4[1]	P1	O2	72.7(6)
O4[1]	P1	O2[1]	107.3(6)
O4	P1	O2[1]	72.7(6)
O2[1]	P1	O2	180.0
O3	P1	O4	68.8(7)
O3	P1	O4[1]	111.2(7)
O3[1]	P1	O4	111.2(7)
O3[1]	P1	O4[1]	68.8(7)
O3[1]	P1	O2	109.3(6)
O3	P1	O2[1]	109.3(6)
O3[1]	P1	O2[1]	70.7(6)
O3	P1	O2	70.7(6)
O3	P1	O3[1]	180.0
O3[1]	P1	O1	68.7(6)
O3	P1	O1[1]	68.7(6)
O3[1]	P1	O1[1]	111.3(6)
O3	P1	O1	111.3(6)
O1[1]	P1	O4	109.3(7)
O1	P1	O4	70.7(7)
O1[1]	P1	O4[1]	70.7(7)
O1	P1	O4[1]	109.3(7)
O1	P1	O2	71.7(7)
O1[1]	P1	O2	108.3(7)
O1[1]	P1	O2[1]	71.7(7)
O1	P1	O2[1]	108.3(7)

Atom	Atom	Atom	Angle/°
O1[1]	P1	O1	180.0
C31	P3	C43	108.0(5)
C31	P3	C37	110.7(5)
C31	P3	C25	110.0(5)
C37	P3	C43	109.6(5)
C25	P3	C43	110.8(5)
C25	P3	C37	107.7(4)
C7	P2	C19	107.2(5)
C7	P2	C13	110.3(5)
C7	P2	C1	108.3(5)
C13	P2	C19	109.7(5)
C1	P2	C19	111.0(5)
C1	P2	C13	110.4(5)
Mo5	O13	Mo1[1]	140.8(4)
Mo6	O11	Mo5	140.1(4)
Mo6	O14	Mo2	139.4(5)
Mo3	O7	Mo2	138.5(4)
Mo4[1]	O16	Mo6	138.7(5)
Mo1[1]	O12	Mo6	138.8(4)
Mo2	O6	Mo1	138.5(5)
Mo4	O8	Mo3	138.8(5)
Mo1	O5	Mo3	139.6(5)
Mo2	O15	Mo4[1]	138.2(4)
Mo3	O10	Mo5	138.2(5)
Mo5	O9	Mo4	138.6(5)
C44	C43	P3	119.2(7)
C44	C43	C48	120.4(9)
C48	C43	P3	120.4(8)
C36	C31	P3	121.2(8)
C32	C31	P3	119.4(8)
C32	C31	C36	118.8(9)
C43	C44	C45	120.3(9)
C42	C37	P3	118.7(8)
C38	C37	P3	122.6(8)
C38	C37	C42	118.7(10)
C27	C26	C25	121.5(10)
C44	C45	C46	119.1(10)
C29	C30	C25	121.2(10)
C24	C19	P2	121.4(8)
C24	C19	C20	119.8(10)
C20	C19	P2	118.7(8)
C26	C25	P3	120.1(8)
C30	C25	P3	123.0(8)
C30	C25	C26	116.5(9)
C28	C27	C26	119.5(10)
C8	C7	P2	122.1(8)
C8	C7	C12	118.8(10)
C12	C7	P2	119.1(8)
C35	C36	C31	119.7(13)
C49	N1	C55	119.8(13)
C56	N1	C49	124.4(13)
C56	N1	C55	115.9(15)
C14	C13	P2	120.1(9)
C14	C13	C18	119.6(11)
C18	C13	P2	120.1(9)
C22	C23	C24	119.7(11)
C33	C32	C31	120.3(11)
C6	C1	P2	117.8(9)
C2	C1	P2	122.3(9)
C2	C1	C6	119.6(11)
C29	C28	C27	120.5(10)
C34	C33	C32	120.1(11)
C33	C34	C35	120.7(11)

Atom	Atom	Atom	Angle/°
C9	C8	C7	120.0(12)
C19	C24	C23	120.6(11)
C47	C48	C43	119.3(10)
C5	C6	C1	120.0(13)
C13	C14	C15	118.9(13)
C47	C46	C45	120.0(10)
C3	C4	C5	120.1(13)
C41	C42	C37	121.0(11)
C23	C22	C21	120.8(12)
Mo6	O4	Mo4[1]	92.4(4)
Mo6	O4	Mo2	93.2(4)
Mo2	O4	Mo4[1]	91.9(4)
P1	O4	Mo6	125.1(7)
P1	O4	Mo4[1]	121.9(7)
P1	O4	Mo2	123.4(7)
C16	C15	C14	121.2(13)
C6	C5	C4	120.6(14)
C40	C41	C42	119.0(12)
C19	C20	C21	119.3(12)
C48	C47	C46	120.9(10)
C37	C38	C39	119.1(11)
C1	C2	C3	118.9(12)
C28	C29	C30	120.7(10)
C39	C40	C41	120.6(12)
C9	C10	C11	120.3(12)
C13	C18	C17	119.8(13)
C4	C3	C2	120.6(14)
C12	C11	C10	120.0(13)
C40	C39	C38	121.5(12)
C15	C16	C17	120.8(12)
C11	C12	C7	120.0(12)
C10	C9	C8	120.6(12)
C36	C35	C34	120.5(13)
C51	C52	C53	120.0
C52	C51	C50	120.0
C49	C50	C51	120.0
C50	C49	N1	121.2(8)
C54	C49	N1	118.8(8)
C54	C49	C50	120.0
C49	C54	C53	120.0

Atom	Atom	Atom	Angle/°
C54	C53	C52	120.0
C16	C17	C18	119.6(14)
O23	C56	N1	126.6(17)
C22	C21	C20	119.5(14)
Mo5	O2	Mo3	93.6(4)
Mo5	O2	Mo4	93.1(4)
Mo3	O2	Mo4	92.6(4)
P1	O2	Mo5	124.7(6)
P1	O2	Mo3	122.7(6)
P1	O2	Mo4	121.7(6)
Mo6	O3	Mo5	91.3(4)
Mo1[1]	O3	Mo6	92.0(4)
Mo1[1]	O3	Mo5	91.5(4)
P1	O3	Mo6	125.0(7)
P1	O3	Mo1[1]	125.2(7)
P1	O3	Mo5	122.2(6)
C57	C58	C59	120.0
C58	C57	C62	120.0
N2	C57	C58	122.0(18)
N2	C57	C62	118.0(18)
C61	C62	C57	120.0
C60	C61	C62	120.0
C61	C60	C59	120.0
C60	C59	C58	120.0
Mo1	O1	Mo3	92.5(4)
Mo1	O1	Mo2	93.1(4)
Mo2	O1	Mo3	91.6(4)
P1	O1	Mo1	124.9(7)
P1	O1	Mo3	122.4(7)
P1	O1	Mo2	123.4(7)
P1	O1	O3[1]	54.5(5)
O3[1]	O1	Mo1	70.5(6)
O3[1]	O1	Mo3	133.6(8)
O3[1]	O1	Mo2	130.8(8)
O24	C64	N2	129(3)
C57	N2	C63	125(2)
C64	N2	C57	121(2)
C64	N2	C63	114(3)

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

Table 5: Torsion Angles in ° for **compound1**.

Atom	Atom	Atom	Atom	Angle/°
P3	C43	C44	C45	178.0(8)
P3	C43	C48	C47	-179.8(9)
P3	C31	C36	C35	-170.4(11)
P3	C31	C32	C33	169.7(8)
P3	C37	C42	C41	177.9(9)
P3	C37	C38	C39	-178.5(10)
P2	C19	C24	C23	179.9(9)
P2	C19	C20	C21	179.6(12)
P2	C7	C8	C9	-178.2(9)
P2	C7	C12	C11	179.1(10)
P2	C13	C14	C15	176.0(9)
P2	C13	C18	C17	-177.0(10)
P2	C1	C6	C5	-177.2(10)
P2	C1	C2	C3	179.0(9)
O20	Mo4	O8	Mo3	-156.2(8)
O18	Mo2	O6	Mo1	156.2(7)
O18	Mo2	O15	Mo4[1]	-152.2(7)
O13[1]	Mo1	O5	Mo3	-12.5(14)

Atom	Atom	Atom	Atom	Angle/°
O13	Mo5	O9	Mo4	101.6(8)
O11	Mo6	O14	Mo2	100.1(7)
O11	Mo5	O13	Mo1[1]	54.4(7)
O11	Mo5	O9	Mo4	13.5(14)
O22	Mo6	O11	Mo5	154.3(7)
O22	Mo6	O14	Mo2	-156.0(7)
O19	Mo3	O7	Mo2	152.2(7)
O19	Mo3	O10	Mo5	-154.2(7)
O14	Mo6	O11	Mo5	-102.6(8)
O14	Mo2	O6	Mo1	-10.3(14)
O14	Mo2	O15	Mo4[1]	-52.7(8)
O7	Mo3	O10	Mo5	102.5(7)
O7	Mo2	O6	Mo1	55.3(7)
O7	Mo2	O15	Mo4[1]	11.9(14)
O16	Mo6	O11	Mo5	-12.4(14)
O16	Mo6	O14	Mo2	-55.8(7)
O16[1]	Mo4	O8	Mo3	100.1(8)
O12	Mo6	O11	Mo5	52.9(8)
O12	Mo6	O14	Mo2	5.6(14)
O12[1]	Mo1	O5	Mo3	-102.6(8)
O6	Mo1	O5	Mo3	54.3(8)
O6	Mo2	O15	Mo4[1]	103.8(8)
O21	Mo5	O13	Mo1[1]	153.3(7)
O21	Mo5	O9	Mo4	-154.3(7)
O8	Mo3	O7	Mo2	-17.0(13)
O8	Mo3	O10	Mo5	-54.2(7)
O5	Mo3	O7	Mo2	51.3(7)
O5	Mo3	O10	Mo5	11.2(13)
O15[1]	Mo4	O8	Mo3	5.0(15)
O15	Mo2	O6	Mo1	-101.1(7)
O10	Mo5	O13	Mo1[1]	-6.9(13)
O10	Mo5	O9	Mo4	-54.1(8)
O10	Mo3	O7	Mo2	-104.3(7)
O9	Mo5	O13	Mo1[1]	-101.7(7)
O9	Mo4	O8	Mo3	-56.2(8)
O17	Mo1	O5	Mo3	154.5(7)
C43	P3	C31	C36	92.2(10)
C43	P3	C31	C32	-78.9(9)
C43	P3	C37	C42	-171.2(8)
C43	P3	C37	C38	8.9(10)
C43	P3	C25	C26	-164.9(8)
C43	P3	C25	C30	23.1(10)
C43	C44	C45	C46	0.1(15)
C43	C48	C47	C46	3.6(17)
C31	P3	C43	C44	-3.6(9)
C31	P3	C43	C48	174.1(8)
C31	P3	C37	C42	69.8(9)
C31	P3	C37	C38	-110.1(9)
C31	P3	C25	C26	-45.5(9)
C31	P3	C25	C30	142.4(8)
C31	C36	C35	C34	1(2)
C31	C32	C33	C34	0.8(16)
C44	C43	C48	C47	-2.1(16)
C44	C45	C46	C47	1.4(16)
C37	P3	C43	C44	-124.3(8)
C37	P3	C43	C48	53.5(10)
C37	P3	C31	C36	-147.8(9)
C37	P3	C31	C32	41.1(9)
C37	P3	C25	C26	75.2(9)
C37	P3	C25	C30	-96.8(9)
C37	C42	C41	C40	1.3(19)
C37	C38	C39	C40	0(2)
C26	C27	C28	C29	0.2(17)

Atom	Atom	Atom	Atom	Angle/°
C45	C46	C47	C48	-3.2(18)
C19	P2	C7	C8	139.7(9)
C19	P2	C7	C12	-41.0(10)
C19	P2	C13	C14	-67.7(10)
C19	P2	C13	C18	107.7(9)
C19	P2	C1	C6	-54.6(10)
C19	P2	C1	C2	131.1(9)
C19	C20	C21	C22	3(2)
C25	P3	C43	C44	117.0(8)
C25	P3	C43	C48	-65.3(10)
C25	P3	C31	C36	-28.9(11)
C25	P3	C31	C32	160.1(8)
C25	P3	C37	C42	-50.5(9)
C25	P3	C37	C38	129.6(9)
C25	C26	C27	C28	-0.2(16)
C25	C30	C29	C28	-1.4(17)
C27	C26	C25	P3	-173.1(8)
C27	C26	C25	C30	-0.6(15)
C27	C28	C29	C30	0.6(18)
C7	P2	C19	C24	138.1(9)
C7	P2	C19	C20	-40.6(10)
C7	P2	C13	C14	174.5(9)
C7	P2	C13	C18	-10.1(11)
C7	P2	C1	C6	62.7(10)
C7	P2	C1	C2	-111.6(9)
C7	C8	C9	C10	0.9(19)
C36	C31	C32	C33	-1.6(15)
N1	C49	C54	C53	178.2(9)
C13	P2	C19	C24	18.4(10)
C13	P2	C19	C20	-160.4(9)
C13	P2	C7	C8	-101.0(9)
C13	P2	C7	C12	78.4(10)
C13	P2	C1	C6	-176.4(9)
C13	P2	C1	C2	9.3(11)
C13	C14	C15	C16	0(2)
C13	C18	C17	C16	2(2)
C23	C22	C21	C20	-6(2)
C32	C31	C36	C35	0.7(18)
C32	C33	C34	C35	1.0(19)
C1	P2	C19	C24	-103.8(9)
C1	P2	C19	C20	77.4(10)
C1	P2	C7	C8	19.9(10)
C1	P2	C7	C12	-160.8(9)
C1	P2	C13	C14	54.9(10)
C1	P2	C13	C18	-129.7(9)
C1	C6	C5	C4	1(2)
C1	C2	C3	C4	-5.2(19)
C33	C34	C35	C36	-2(2)
C8	C7	C12	C11	-1.5(18)
C24	C19	C20	C21	0.9(19)
C24	C23	C22	C21	5(2)
C48	C43	C44	C45	0.3(15)
C6	C1	C2	C3	4.9(16)
C14	C13	C18	C17	-1.6(17)
C14	C15	C16	C17	1(2)
C42	C37	C38	C39	1.6(17)
C42	C41	C40	C39	0(2)
C22	C23	C24	C19	-1.7(18)
O4	Mo6	O11	Mo5	-38.0(8)
O4	Mo6	O14	Mo2	7.1(7)
O4[1]	Mo4	O8	Mo3	35.6(8)
O4	Mo2	O6	Mo1	-35.3(8)
O4	Mo2	O15	Mo4[1]	8.3(7)

Atom	Atom	Atom	Atom	Angle/°
O4	P1	O2	Mo5	63.4(9)
O4[1]	P1	O2	Mo5	-116.6(9)
O4	P1	O2	Mo3	-58.9(8)
O4[1]	P1	O2	Mo3	121.1(8)
O4[1]	P1	O2	Mo4	3.8(7)
O4	P1	O2	Mo4	-176.2(7)
O4	P1	O3	Mo6	-3.9(7)
O4[1]	P1	O3	Mo6	176.1(7)
O4[1]	P1	O3	Mo1[1]	-60.9(9)
O4	P1	O3	Mo1[1]	119.1(9)
O4[1]	P1	O3	Mo5	57.9(9)
O4	P1	O3	Mo5	-122.1(9)
O4	P1	O1	Mo1	-126.2(10)
O4[1]	P1	O1	Mo1	53.8(10)
O4[1]	P1	O1	Mo3	-66.6(9)
O4	P1	O1	Mo3	113.4(9)
O4[1]	P1	O1	Mo2	176.3(7)
O4	P1	O1	Mo2	-3.7(7)
O4	P1	O1	O3[1]	-123.2(8)
O4[1]	P1	O1	O3[1]	56.8(8)
C15	C16	C17	C18	-2(2)
C5	C4	C3	C2	3(2)
C41	C40	C39	C38	-1(2)
C20	C19	C24	C23	-1.4(17)
C38	C37	C42	C41	-2.2(17)
C2	C1	C6	C5	-2.8(18)
C29	C30	C25	P3	173.6(8)
C29	C30	C25	C26	1.3(15)
C10	C11	C12	C7	-3(2)
C18	C13	C14	C15	0.6(17)
C3	C4	C5	C6	-1(2)
C11	C10	C9	C8	-5(2)
C12	C7	C8	C9	2.5(17)
C9	C10	C11	C12	6(2)
C52	C51	C50	C49	0.0
C51	C52	C53	C54	0.0
C51	C50	C49	N1	-178.2(10)
C51	C50	C49	C54	0.0
C50	C49	C54	C53	0.0
C49	N1	C56	O23	177.5(13)
C49	C54	C53	C52	0.0
C53	C52	C51	C50	0.0
C56	N1	C49	C50	-5.1(17)
C56	N1	C49	C54	176.7(12)
C55	N1	C49	C50	175.8(16)
C55	N1	C49	C54	-2.5(19)
C55	N1	C56	O23	-3(3)
O2	Mo5	O13	Mo1[1]	-36.1(8)
O2	Mo5	O9	Mo4	7.9(7)
O2	Mo3	O7	Mo2	-40.6(7)
O2	Mo3	O10	Mo5	8.0(6)
O2	Mo4	O8	Mo3	4.7(7)
O2	P1	O4	Mo6	-56.5(9)
O2[1]	P1	O4	Mo6	123.5(9)
O2	P1	O4	Mo4[1]	-176.3(7)
O2[1]	P1	O4	Mo4[1]	3.7(7)
O2[1]	P1	O4	Mo2	-113.5(9)
O2	P1	O4	Mo2	66.5(9)
O2	P1	O3	Mo6	114.4(9)
O2[1]	P1	O3	Mo6	-65.6(9)
O2[1]	P1	O3	Mo1[1]	57.4(9)
O2	P1	O3	Mo1[1]	-122.6(9)
O2	P1	O3	Mo5	-3.8(6)

Atom	Atom	Atom	Atom	Angle/°
O2[1]	P1	O3	Mo5	176.2(6)
O2	P1	O1	Mo1	117.1(9)
O2[1]	P1	O1	Mo1	-62.9(9)
O2	P1	O1	Mo3	-3.2(6)
O2[1]	P1	O1	Mo3	176.8(6)
O2	P1	O1	Mo2	-120.3(9)
O2[1]	P1	O1	Mo2	59.7(9)
O2	P1	O1	O3[1]	120.2(7)
O2[1]	P1	O1	O3[1]	-59.8(7)
O3	Mo6	O11	Mo5	-8.3(7)
O3	Mo6	O14	Mo2	34.7(8)
O3[1]	Mo1	O5	Mo3	-37.8(8)
O3	Mo5	O13	Mo1[1]	-7.2(7)
O3	Mo5	O9	Mo4	38.1(8)
O3[1]	P1	O4	Mo6	-176.0(7)
O3	P1	O4	Mo6	4.0(7)
O3	P1	O4	Mo4[1]	-115.8(9)
O3[1]	P1	O4	Mo4[1]	64.2(9)
O3[1]	P1	O4	Mo2	-53.0(9)
O3	P1	O4	Mo2	127.0(9)
O3[1]	P1	O2	Mo5	-175.9(7)
O3	P1	O2	Mo5	4.1(7)
O3	P1	O2	Mo3	-118.2(8)
O3[1]	P1	O2	Mo3	61.8(8)
O3[1]	P1	O2	Mo4	-55.5(9)
O3	P1	O2	Mo4	124.5(9)
O3[1]	P1	O1	Mo1	-3.0(7)
O3	P1	O1	Mo1	177.0(7)
O3[1]	P1	O1	Mo3	-123.4(9)
O3	P1	O1	Mo3	56.6(9)
O3	P1	O1	Mo2	-60.5(9)
O3[1]	P1	O1	Mo2	119.5(9)
O3	P1	O1	O3[1]	180.002(3)
O24	C64	N2	C57	175(4)
O24	C64	N2	C63	1(6)
C58	C57	C62	C61	0.0
C58	C57	N2	C63	-156(3)
C58	C57	N2	C64	32(4)
C57	C58	C59	C60	0.0
C57	C62	C61	C60	0.0
C62	C57	N2	C63	24(4)
C62	C57	N2	C64	-148(3)
C62	C61	C60	C59	0.0
C61	C60	C59	C58	0.0
C59	C58	C57	C62	0.0
C59	C58	C57	N2	-180(3)
O1	Mo1	O5	Mo3	-8.3(7)
O1	Mo3	O7	Mo2	-8.9(6)
O1	Mo3	O10	Mo5	37.4(8)
O1	Mo2	O6	Mo1	-7.0(6)
O1	Mo2	O15	Mo4[1]	39.5(8)
O1	P1	O4	Mo6	-119.3(9)
O1[1]	P1	O4	Mo6	60.7(9)
O1	P1	O4	Mo4[1]	121.0(9)
O1[1]	P1	O4	Mo4[1]	-59.0(9)
O1	P1	O4	Mo2	3.7(7)
O1[1]	P1	O4	Mo2	-176.3(7)
O1	P1	O2	Mo5	125.5(9)
O1[1]	P1	O2	Mo5	-54.5(9)
O1[1]	P1	O2	Mo3	-176.8(6)
O1	P1	O2	Mo3	3.2(6)
O1	P1	O2	Mo4	-114.1(8)
O1[1]	P1	O2	Mo4	65.9(8)

Atom	Atom	Atom	Atom	Angle/°
O1[1]	P1	O3	Mo6	-126.0(10)
O1	P1	O3	Mo6	54.0(10)
O1[1]	P1	O3	Mo1[1]	-3.0(7)
O1	P1	O3	Mo1[1]	177.0(7)
O1[1]	P1	O3	Mo5	115.8(9)
O1	P1	O3	Mo5	-64.2(9)
N2	C57	C62	C61	180(3)

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

Table 6: Hydrogen Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **compound1**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H44	8334.85	7265.73	3650.26	51
H26	4625.38	7345.22	4554.01	51
H45	10158.53	6490.97	3169.84	57
H30	7187.97	4883.54	4006.91	56
H27	3796.45	6538.73	4172.88	62
H36	6119.69	7782.01	3276.27	73
H23	2116.23	7723.17	1997.19	72
H32	6451.31	8586.23	5357.28	55
H28	4676.08	4918.74	3696.95	65
H33	6392.68	10052.92	4783.28	71
H34	6204.73	10380.18	3478.42	84
H8	1704.54	3734.54	-175.5	63
H24	1129.32	7254.13	1475.05	63
H48	7993.76	4957.6	4957.02	60
H6	2164.04	3808.65	1494.3	77
H14	-498.63	7020.23	1743.4	75
H46	10886.09	4939.71	3592.75	66
H4	-307.98	3096.87	2856.1	106
H42	4496.92	7414.04	6009.07	65
H22	3680.51	6592.07	2016.97	81
H15	-1692.48	8419.53	1455.84	92
H5	1460.16	2797.53	2404.6	96
H41	3714.72	7419.21	7504.81	78
H20	3406.02	4576.06	795.47	78
H47	9803.33	4156.43	4419.65	69
H38	7346.63	6344.74	6131.4	69
H2	-687.79	5444.32	1464.81	67
H29	6349.71	4110.86	3602.84	65
H40	4754.14	6899.8	8305.05	79
H10	4308.79	3222.83	-2339.9	94
H18	1110.49	6360.13	-847.57	71
H3	-1392.76	4451.92	2462.51	92
H11	4332.33	4702.7	-2069.22	95
H39	6531.58	6382.81	7630.05	88
H16	-1493.6	8782.98	62.89	95
H12	3149.28	5623.33	-769.27	77
H9	2933.6	2811.95	-1465.45	81
H35	6022.77	9269.27	2745.75	106
H52	5575.11	11181.19	1727.96	132
H51	6973.12	10226.82	510.16	171
H50	6830.28	8979.16	-102.42	141
H54	3891.41	9640.22	1720.59	106
H53	4034.23	10887.89	2333.18	128
H17	-137.55	7748.8	-1098.11	99
H56	6538.53	8018.05	-582.78	101
H21	4408.69	5066.88	1307.06	125
H55A	4104.59	8227.11	1462.65	277
H55B	4418.28	7574.78	632.43	277

Atom	x	y	z	U_{eq}
H55C	3721.67	8688.34	713.75	277
H58	385.91	9663.13	11033.1	106
H62	-292.42	10321.58	8891.18	90
H61	-1952	11437.57	9741.44	118
H60	-2442.65	11666.36	11237.54	121
H59	-1273.71	10779.15	11883.38	108
H63A	1520.89	8897.06	8142.24	153
H63B	2430.46	9038.13	8296.12	153
H63C	1433.55	9946.49	8317.94	153
H64	1358.79	8365.57	10239.03	97

Table 7: Atomic Occupancies for all atoms that are not fully occupied in **compound1**.

Atom	Occupancy
O4	0.5
O2	0.5
O3	0.5
O24	0.5
C58	0.5
H58	0.5
C57	0.5
C62	0.5
H62	0.5
C61	0.5
H61	0.5
C60	0.5
H60	0.5
C59	0.5
H59	0.5
O1	0.5
C63	0.5
H63A	0.5
H63B	0.5
H63C	0.5
C64	0.5
H64	0.5
N2	0.5

Citations

O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.

SADABS, Bruker axs, Madison, WI (?).

SAINT - Software for the Integration of CCD Detector System Bruker Analytical X-ray Systems, Bruker axs, Madison, WI (?).

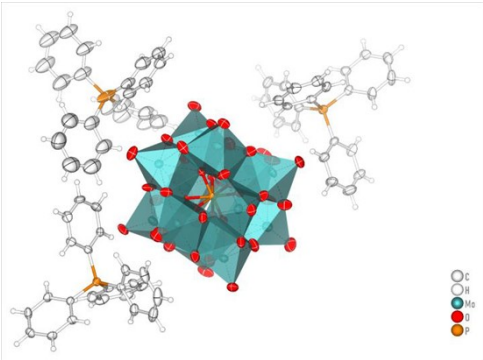
Sheldrick, G.M., Crystal structure refinement with ShelXL, *Acta Cryst.*, (2015), **C71**, 3-8.

Sheldrick, G.M., ShelXT-Integrated space-group and crystal-structure determination, *Acta Cryst.*, (2015), **A71**, 3-8.

Compound 2

R_1=5.30%

Crystal Data and Experimental



Compound	**comp-2_sg**
Formula	$C_{86}H_{75.75}Mo_{12}N_{1.75}O_{41.75}P_4$
$D_{calc.}$/ g cm-3	2.108
μ/mm^{-1}	1.653
Formula Weight	3076.89
Colour	clear yellow
Shape	plate-shaped
Size/mm3	0.20.0.18.0.17
T/*K*	100(2)
Crystal System	monoclinic
Space Group	*P21/n*
a/*Å*	14.219(3)
b/*Å*	25.074(6)
c/*Å*	27.423(7)
α/°	90
β/°	97.437(11)
γ/°	90
V/Å^3	9695(4)
Z	4
Z'	1
Wavelength/Å	0.71073
Radiation type	MoK□
Θ_{min}/°	2.105
Θ_{max}/°	24.999
Measured Refl's.	317477
Indep't Refl's	17041
Refl's I≥2 □(I)	12616
Rint	0.1447
Parameters	1190
Restraints	360
Largest Peak	1.107
Deepest Hole	-1.129
GooF	1.034
wR2 (all data)	0.1104
wR2	0.0996
R1 (all data)	0.0795
R1	0.0530

Experimental. Single clear yellow plate-shaped crystals of **comp-2_sg** recrystallised from a mixture of water and methanol by slow evaporation. A suitable crystal with dimensions 0.20 × 0.18 × 0.17 mm^3 was selected and mounted on a Bruker APEX-II CCD diffractometer. The crystal was kept at a steady *T* = 100(2) K during data collection. The structure was solved with the Superflip (Palatinus & Chapuis, 2007;Palatinus & van der Lee, 2008;Palatinus et al., 2012) solution program using ? and by using Olex2 1.5-dev (Dolomanov et al., 2009) as the graphical interface. The model was refined with ShelXL 2018/3 (Sheldrick, 2015) using full matrix least squares minimisation on F^2.

Crystal Data. $C_{86}H_{75.75}Mo_{12}N_{1.75}O_{41.75}P_4$, M_r = 3076.89, monoclinic, $P2_1/n$ (No. 14), a = 14.219(3) Å, b = 25.074(6) Å, c = 27.423(7) Å, □□= 97.437(11)°, □□= □□= 90°, *V* = 9695(4) Å^3, *T* = 100(2) K, *Z* = 4, *Z'* = 1, □□ (MoK$_\alpha$) = 1.653, 317477 reflections measured, 17041 unique (R_{int} = 0.1447) which were used in all calculations. The final wR_2 was 0.1104 (all data) and R_1 was 0.0530 (I≥2σ(I)).

Structure Quality Indicators

Reflections:	d min (Mo) 2Θ=50.0° 0.84	I/σ(I) 19.0	Rint m=18.91 14.47%	Full 50.0° 99.9
Refinement:	Shift 0.002	Max Peak 1.1	Min Peak -1.1	GooF 1.034

A clear yellow plate-shaped-shaped crystal with dimensions 0.20 × 0.18 × 0.17 mm^3 was mounted. Data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature device operating at T = 100(2) K.

Data were measured using ϕ and ω scans with MoK_α radiation. . The maximum resolution that was achieved was Θ = 24.999° (0.84 Å).

The unit cell was refined using SAINT v8.37A (Bruker, 2015) on 9634 reflections, 3% of the observed reflections.

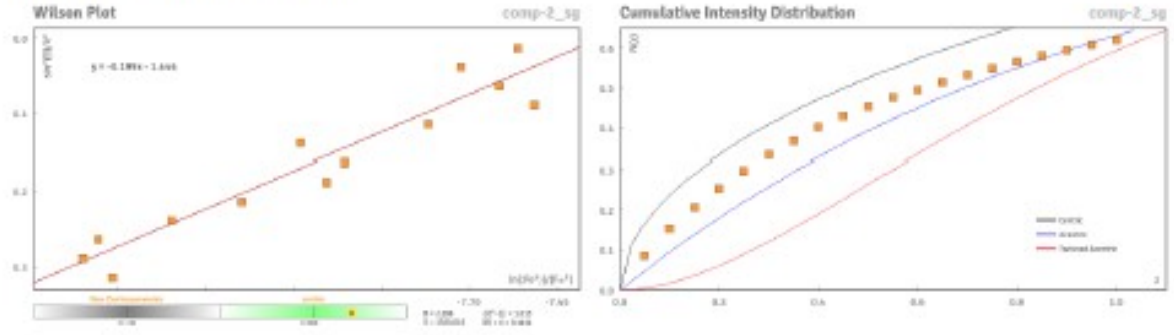
Data reduction, scaling and absorption corrections were performed using SAINT v8.37A (Bruker, 2015). The final completeness is 99.90 % out to 24.999° in Θ. No absorption correction was performed. The absorption coefficient μ of this material is 1.653 mm^{-1} at this wavelength (λ = 0.71073Å) and the minimum and maximum transmissions are 0.064 and 0.096.

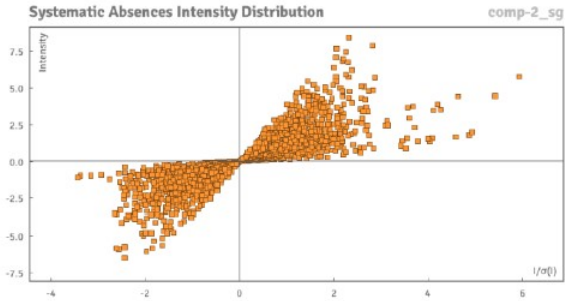
The structure was solved and the space group $P2_1/n$ (# 14) determined by the Superflip (Palatinus & Chapuis, 2007;Palatinus & van der Lee, 2008;Palatinus et al., 2012) structure solution program using using ? and refined by full matrix least squares minimisation on F^2 using version 2018/3 of ShelXL 2018/3 (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model.

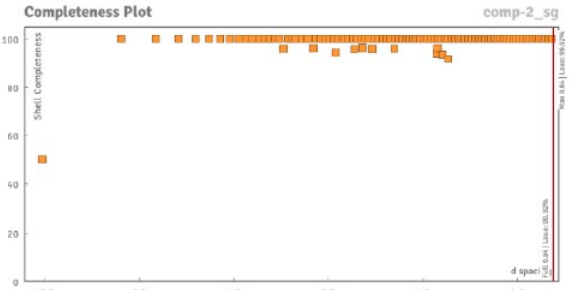
_exptl_absorpt_process_details: SADABS-2008/1 (Bruker,2008) was used for absorption correction.wR_2(int) was 0.1105 before and 0.0997 after correction.The Ratio of minimum to maximum transmission is 0.6632.The $\lambda/2$ correction factor is 0.0015.

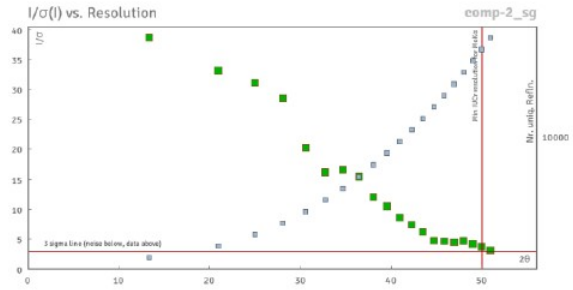
_smtbx_masks_special_details: A solvent mask was calculated and 506 electrons were found in a volume of 1558Å^3 in 2 voids per unit cell. This is consistent with the presence of 1.75[C8H9NO] per Formula Unit (7*N-Methyl Formanilide per unit cell) which account for 504 electrons per unit cell.

Data Plots: Diffraction Data

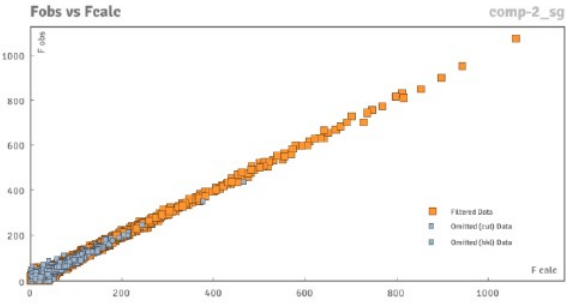








Data Plots: Refinement and Data



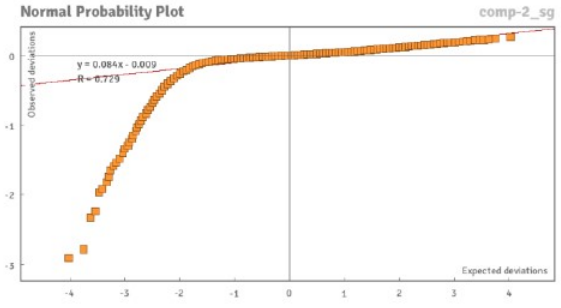


Table 8: Bond Lengths in Å for **compound2**.

Atom	Atom	Length/Å
Mo5	O9	1.839(5)
Mo5	O12	1.807(5)
Mo5	O11	2.030(6)
Mo5	O14	2.011(5)
Mo5	O1	2.437(5)
Mo5	O37	1.657(5)
Mo5	O2	2.51(2)
Mo1	O33	1.671(6)
Mo1	O13	1.825(5)
Mo1	O12	1.995(5)
Mo1	O15	2.008(5)
Mo1	O17	1.823(5)
Mo1	O3	2.429(6)
Mo1	O2	2.42(2)
Mo3	O16	1.997(5)
Mo3	O15	1.844(6)
Mo3	O19	1.995(6)
Mo3	O3	2.480(6)
Mo3	O18	1.812(5)
Mo3	O35	1.666(5)
Mo3	O4	2.49(3)
Mo6	O38	1.673(5)
Mo6	O20	1.825(5)

Atom	Atom	Length/Å
Mo6	O9	2.008(5)
Mo6	O18	1.993(5)
Mo6	O10	1.838(6)
Mo6	O1	2.458(6)
Mo6	O4	2.55(2)
Mo2	O16	1.843(5)
Mo2	O24	2.006(5)
Mo2	O17	2.018(6)
Mo2	O3	2.456(6)
Mo2	O26	1.798(6)
Mo2	O34	1.657(5)
Mo2	O6	2.38(3)
Mo10	O42	1.671(5)
Mo10	O20	1.988(5)
Mo10	O21	1.839(6)
Mo10	O23	2.009(6)
Mo10	O19	1.798(6)
Mo10	O5	2.441(6)
Mo10	O4	2.41(2)
Mo9	O41	1.671(6)
Mo9	O30	1.997(5)
Mo9	O29	1.834(6)
Mo9	O28	2.016(6)

Atom	Atom	Length/Å
Mo9	O32	1.801(6)
Mo9	O7	2.446(5)
Mo9	O8	2.55(3)
Mo4	O36	1.649(5)
Mo4	O11	1.840(6)
Mo4	O30	1.819(6)
Mo4	O31	1.989(5)
Mo4	O10	2.038(6)
Mo4	O1	2.434(5)
Mo4	O8	2.57(3)
Mo8	O40	1.677(5)
Mo8	O13	1.978(5)
Mo8	O14	1.807(5)
Mo8	O27	2.028(6)
Mo8	O28	1.843(6)
Mo8	O7	2.436(6)
Mo8	O2	2.58(2)
Mo11	O43	1.677(5)
Mo11	O21	2.002(6)

Atom	Atom	Length/Å
Mo11	O26	1.990(6)
Mo11	O22	1.835(6)
Mo11	O25	1.794(6)
Mo11	O5	2.464(6)
Mo11	O6	2.47(3)
Mo12	O23	1.850(6)
Mo12	O22	2.002(6)
Mo12	O31	1.818(6)
Mo12	O44	1.678(6)
Mo12	O32	2.011(6)
Mo12	O5	2.441(6)
Mo12	O8	2.49(3)
Mo7	O24	1.803(6)
Mo7	O29	2.005(6)
Mo7	O27	1.829(6)
Mo7	O39	1.669(5)
Mo7	O25	2.010(6)
Mo7	O7	2.445(6)
Mo7	O6	2.52(3)

Table 9: Bond Angles in ˚ for **compound 2**.

Atom	Atom	Atom	Angle/˚
O9	Mo5	O11	86.9(2)
O9	Mo5	O14	154.7(2)
O9	Mo5	O1	72.7(2)
O9	Mo5	O2	103.3(6)
O12	Mo5	O9	97.9(2)
O12	Mo5	O11	155.1(3)
O12	Mo5	O14	86.0(2)
O12	Mo5	O1	88.5(2)
O12	Mo5	O2	55.7(6)
O11	Mo5	O1	69.5(2)
O11	Mo5	O2	99.4(6)
O14	Mo5	O11	79.8(2)
O14	Mo5	O1	82.5(2)
O14	Mo5	O2	58.5(6)
O37	Mo5	O9	102.5(3)
O37	Mo5	O12	104.4(3)
O37	Mo5	O11	98.4(3)
O37	Mo5	O14	100.7(3)
O37	Mo5	O1	166.9(2)
O37	Mo5	O2	149.3(6)
O33	Mo1	O13	103.6(3)
O33	Mo1	O12	101.9(3)
O33	Mo1	O15	99.7(3)
O33	Mo1	O17	102.5(3)
O33	Mo1	O3	168.3(3)
O33	Mo1	O2	150.3(6)
O13	Mo1	O12	85.9(2)
O13	Mo1	O15	154.8(3)
O13	Mo1	O3	87.5(2)
O13	Mo1	O2	59.2(6)
O12	Mo1	O15	79.9(2)
O12	Mo1	O3	82.3(2)
O12	Mo1	O2	56.0(6)
O15	Mo1	O3	70.1(2)
O15	Mo1	O2	95.6(6)
O17	Mo1	O13	96.9(2)
O17	Mo1	O12	154.0(3)
O17	Mo1	O15	87.3(2)
O17	Mo1	O3	72.0(2)
O17	Mo1	O2	103.5(6)
O16	Mo3	O3	69.0(2)
O16	Mo3	O4	95.1(6)
O15	Mo3	O16	86.7(2)
O15	Mo3	O19	152.9(2)
O15	Mo3	O3	71.2(2)
O15	Mo3	O4	105.0(6)
O19	Mo3	O16	79.1(2)
O19	Mo3	O3	82.1(2)
O19	Mo3	O4	54.1(6)
O18	Mo3	O16	154.0(3)
O18	Mo3	O15	97.6(3)
O18	Mo3	O19	86.0(2)
O18	Mo3	O3	88.0(2)
O18	Mo3	O4	59.0(6)
O35	Mo3	O16	99.1(2)
O35	Mo3	O15	101.9(3)
O35	Mo3	O19	103.1(3)
O35	Mo3	O3	166.2(2)
O35	Mo3	O18	105.0(3)
O35	Mo3	O4	150.1(6)
O38	Mo6	O20	104.1(3)
O38	Mo6	O9	99.1(2)
O38	Mo6	O18	102.0(3)
O38	Mo6	O10	101.5(3)
O38	Mo6	O1	166.9(2)
O38	Mo6	O4	148.6(6)
O20	Mo6	O9	155.1(2)
O20	Mo6	O18	85.9(2)
O20	Mo6	O10	97.4(3)
O20	Mo6	O1	88.1(2)
O20	Mo6	O4	56.3(6)
O9	Mo6	O1	69.7(2)
O9	Mo6	O4	98.9(6)
O18	Mo6	O9	80.5(2)
O18	Mo6	O1	83.3(2)
O18	Mo6	O4	56.3(6)
O10	Mo6	O9	86.6(2)
O10	Mo6	O18	154.7(3)

Atom	Atom	Atom	Angle/°
O10	Mo6	O1	71.8(2)
O10	Mo6	O4	105.1(6)
O16	Mo2	O24	153.4(2)
O16	Mo2	O17	86.9(2)
O16	Mo2	O3	71.7(2)
O16	Mo2	O6	103.9(7)
O24	Mo2	O17	79.5(2)
O24	Mo2	O3	82.0(2)
O24	Mo2	O6	56.1(7)
O17	Mo2	O3	68.6(2)
O17	Mo2	O6	97.3(7)
O26	Mo2	O16	97.8(3)
O26	Mo2	O24	85.4(2)
O26	Mo2	O17	154.0(3)
O26	Mo2	O3	88.5(2)
O26	Mo2	O6	56.7(7)
O34	Mo2	O16	101.9(3)
O34	Mo2	O24	102.7(3)
O34	Mo2	O17	98.9(3)
O34	Mo2	O3	165.9(3)
O34	Mo2	O26	105.0(3)
O34	Mo2	O6	150.1(7)
O42	Mo10	O20	101.1(3)
O42	Mo10	O21	102.5(3)
O42	Mo10	O23	98.5(3)
O42	Mo10	O19	104.2(3)
O42	Mo10	O5	166.7(3)
O42	Mo10	O4	149.9(6)
O20	Mo10	O23	79.7(2)
O20	Mo10	O5	82.8(2)
O20	Mo10	O4	57.8(6)
O21	Mo10	O20	154.1(3)
O21	Mo10	O23	86.6(2)
O21	Mo10	O5	71.8(2)
O21	Mo10	O4	103.3(6)
O23	Mo10	O5	69.5(2)
O23	Mo10	O4	98.2(6)
O19	Mo10	O20	86.7(2)
O19	Mo10	O21	97.6(3)
O19	Mo10	O23	155.4(3)
O19	Mo10	O5	88.6(2)
O19	Mo10	O4	57.2(6)
O41	Mo9	O30	101.4(3)
O41	Mo9	O29	102.6(3)
O41	Mo9	O28	100.3(3)
O41	Mo9	O32	102.9(3)
O41	Mo9	O7	168.1(3)
O41	Mo9	O8	150.4(7)
O30	Mo9	O28	80.2(2)
O30	Mo9	O7	83.1(2)
O30	Mo9	O8	58.9(6)
O29	Mo9	O30	154.2(3)
O29	Mo9	O28	86.3(2)
O29	Mo9	O7	71.6(2)
O29	Mo9	O8	101.9(6)
O28	Mo9	O7	69.3(2)
O28	Mo9	O8	97.7(6)
O32	Mo9	O30	86.1(2)
O32	Mo9	O29	97.6(3)
O32	Mo9	O28	154.9(3)
O32	Mo9	O7	88.3(2)
O32	Mo9	O8	57.3(6)
O36	Mo4	O11	102.0(3)
O36	Mo4	O30	104.3(3)
O36	Mo4	O31	101.4(3)
O36	Mo4	O10	97.7(3)
O36	Mo4	O1	166.0(2)
O36	Mo4	O8	150.3(6)
O11	Mo4	O31	154.2(3)
O11	Mo4	O10	86.0(2)
O11	Mo4	O1	72.3(2)
O11	Mo4	O8	104.9(6)
O30	Mo4	O11	98.1(2)
O30	Mo4	O31	86.5(2)
O30	Mo4	O10	156.1(2)
O30	Mo4	O1	89.3(2)
O30	Mo4	O8	59.7(6)
O31	Mo4	O10	80.2(2)
O31	Mo4	O1	82.4(2)
O31	Mo4	O8	55.7(6)
O10	Mo4	O1	69.4(2)
O10	Mo4	O8	96.5(6)
O40	Mo8	O13	100.9(3)
O40	Mo8	O14	104.0(3)
O40	Mo8	O27	98.3(3)
O40	Mo8	O28	102.7(3)
O40	Mo8	O7	167.3(2)
O40	Mo8	O2	147.8(6)
O13	Mo8	O27	80.2(2)
O13	Mo8	O7	82.7(2)
O13	Mo8	O2	54.7(6)
O14	Mo8	O13	86.4(2)
O14	Mo8	O27	155.8(3)
O14	Mo8	O28	97.7(3)
O14	Mo8	O7	88.3(2)
O14	Mo8	O2	58.5(5)
O27	Mo8	O7	70.1(2)
O27	Mo8	O2	97.4(5)
O28	Mo8	O13	154.3(3)
O28	Mo8	O27	86.3(2)
O28	Mo8	O7	72.1(2)
O28	Mo8	O2	106.2(6)
O43	Mo11	O21	99.3(3)
O43	Mo11	O26	101.7(3)
O43	Mo11	O22	102.6(3)
O43	Mo11	O25	104.3(3)
O43	Mo11	O5	166.8(3)
O43	Mo11	O6	147.6(7)
O21	Mo11	O5	69.0(2)
O21	Mo11	O6	96.1(7)
O26	Mo11	O21	79.7(2)
O26	Mo11	O5	82.6(2)
O26	Mo11	O6	53.5(6)
O22	Mo11	O21	86.3(3)
O22	Mo11	O26	153.6(3)
O22	Mo11	O5	71.5(2)
O22	Mo11	O6	106.7(7)
O25	Mo11	O21	154.6(3)
O25	Mo11	O26	86.4(2)
O25	Mo11	O22	97.5(3)
O25	Mo11	O5	88.4(2)
O25	Mo11	O6	58.7(7)
O23	Mo12	O22	87.0(3)
O23	Mo12	O32	154.4(3)
O23	Mo12	O5	71.8(2)
O23	Mo12	O8	102.6(6)

Atom	Atom	Atom	Angle/°
O22	Mo12	O32	80.6(3)
O22	Mo12	O5	69.6(2)
O22	Mo12	O8	95.3(6)
O31	Mo12	O23	96.9(3)
O31	Mo12	O22	154.1(3)
O31	Mo12	O32	85.3(2)
O31	Mo12	O5	87.2(2)
O31	Mo12	O8	58.8(6)
O44	Mo12	O23	102.6(3)
O44	Mo12	O22	99.3(3)
O44	Mo12	O31	104.8(3)
O44	Mo12	O32	101.5(3)
O44	Mo12	O5	167.5(3)
O44	Mo12	O8	151.4(6)
O32	Mo12	O5	82.9(2)
O32	Mo12	O8	56.9(6)
O24	Mo7	O29	154.6(3)
O24	Mo7	O27	98.4(3)

Atom	Atom	Atom	Angle/°
O24	Mo7	O25	85.5(2)
O24	Mo7	O7	88.5(2)
O24	Mo7	O6	54.9(6)
O29	Mo7	O25	79.9(2)
O29	Mo7	O7	69.2(2)
O29	Mo7	O6	99.7(6)
O27	Mo7	O29	86.8(3)
O27	Mo7	O25	155.1(3)
O27	Mo7	O7	72.8(2)
O27	Mo7	O6	106.4(7)
O39	Mo7	O24	104.2(3)
O39	Mo7	O29	98.9(3)
O39	Mo7	O27	102.3(3)
O39	Mo7	O25	100.5(3)
O39	Mo7	O7	167.0(2)
O39	Mo7	O6	146.4(7)
O25	Mo7	O7	82.8(2)
O25	Mo7	O6	56.0(6)

Citations

L. Palatinus and G. Chapuis, Superflip - a computer program for the solution of crystal structures by charge flipping in arbitrary dimensions, *J. Appl. Cryst.*, (2007), **40**, 786-790.

O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.

SADABS, Bruker axs, Madison, WI (?).

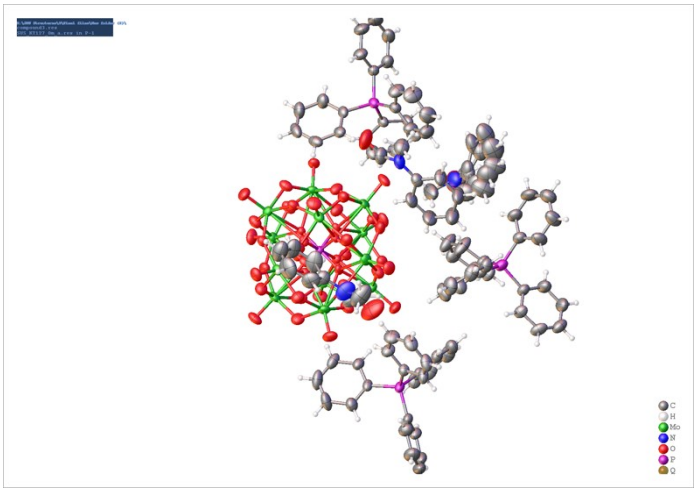
SAINT - Software for the Integration of CCD Detector System Bruker Analytical X-ray Systems, Bruker axs, Madison, WI (?).

Sheldrick, G.M., Crystal structure refinement with ShelXL, *Acta Cryst.*, (2015), **C71**, 3-8.

compound3

R_1=4.76

Crystal Data and Experimental



Experimental. Single clear light orange plate-shaped crystals of **compound3** recrystallised from N-Methyl Formanilide by slow evaporation. A suitable crystal with dimensions 0.20 × 0.18 × 0.17 mm^3 was selected and mounted on a Bruker APEX-II CMOS detector diffractometer. The crystal was kept at a steady T = 292(2) K during data collection. The structure was solved with the ShelXT 2014/4 (Sheldrick, 2014) solution program using iterative methods and by using Olex2 1.5-alpha (Dolomanov et al., 2009) as the graphical interface. The model was refined with ShelXL 2018/3 (Sheldrick, 2015) using full matrix least squares minimisation on F^2.

Crystal Data. $C_{88}H_{78}Mo_{12}N_2O_{42}P_4$, M_r = 3110.68, triclinic, P-1 (No. 2), a = 14.6105(11) Å, b = 15.5593(11) Å, c = 22.6072(16) Å, α = 89.026(3)°, β = 88.285(4)°, γ = 82.439(3)°, V = 5091.9(6) Å^3, T = 292(2) K, Z = 2, Z' = 1, μ(MoK$_\alpha$) = 1.575, 215632 reflections measured, 25302 unique (R_{int} = 0.0504) which were used in all calculations. The final wR_2 was 0.1080 (all data) and R_1 was 0.0476 (I≥2 σ(I)).

Compound	**compound3**
Formula	$C_{88}H_{78}Mo_{12}N_2O_{42}P_4$
$D_{calc.}$/ g cm^{-3}	2.029
μ/mm^{-1}	1.575
Formula Weight	3110.68
Colour	clear light orange
Shape	plate-shaped
Size/mm^3	0.20×0.18×0.17
T/K	292(2)
Crystal System	triclinic
Space Group	P-1
a/Å	14.6105(11)
b/Å	15.5593(11)
c/Å	22.6072(16)
α/°	89.026(3)
β/°	88.285(4)
γ/°	82.439(3)
V/Å^3	5091.9(6)
Z	2
Z'	1
Wavelength/Å	0.71073
Radiation type	MoK$_\alpha$
Θ_{min}/°	2.221
Θ_{max}/°	28.332
Measured Refl's.	215632
Indep't Refl's	25302
Refl's I≥2 σ(I)	18691
R_{int}	0.0504
Parameters	1504
Restraints	971
Largest Peak	2.002
Deepest Hole	-1.696
GooF	1.020
wR_2 (all data)	0.1080
wR_2	0.0964
R_1 (all data)	0.0720
R_1	0.0476

Structure Quality Indicators

Reflections:	d min (Mo) 2Θ=56.7° 0.75	I/σ(I) 32.5	Rint 5.04%	Full 50.5° 99.9
Refinement:	Shift -0.001	Max Peak 2.0	Min Peak -1.7	GooF 1.020

A clear light orange plate-shaped-shaped crystal with dimensions 0.20 × 0.18 × 0.17 mm^3 was mounted. Data were collected using a Bruker APEX-II CMOS detector diffractometer operating at T = 292(2) K.

Data were measured using phi and omega scans with MoK_α radiation. . The maximum resolution that was achieved was Θ = 28.332˚ (0.75 Å).

The unit cell was refined on 9580 reflections, 4% of the observed reflections.

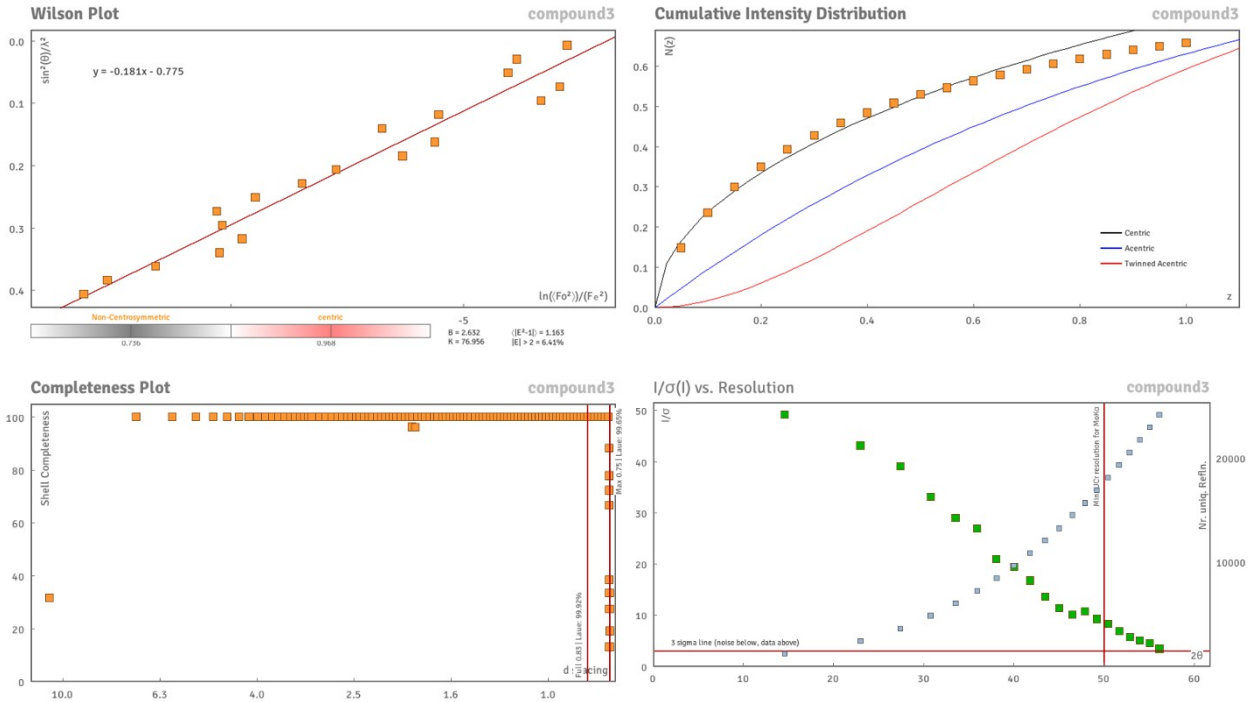
Data reduction, scaling and absorption corrections were performed. The final completeness is 99.90 % out to 28.332˚ in Θ. SADABS-2008/1 (Bruker, 2008) was used for absorption correction. The absorption coefficient μ of this material is 1.575 mm^{-1} at this wavelength (λ = 0.71073Å) and the minimum and maximum transmissions are 0.065 and 0.096.

The structure was solved and the space group P-1 (# 2) determined by the ShelXT 2014/4 (Sheldrick, 2014) structure solution program using using iterative methods and refined by full matrix least squares minimisation on F^2 using version 2018/3 of ShelXL 2018/3 (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model.

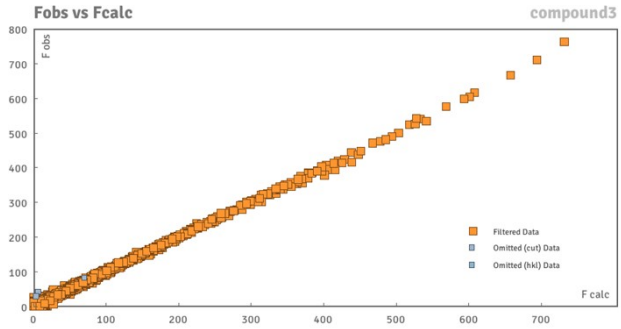
_*exptl_absorpt_process_details*: SADABS-2008/1 (Bruker,2008) was used for absorption correction.

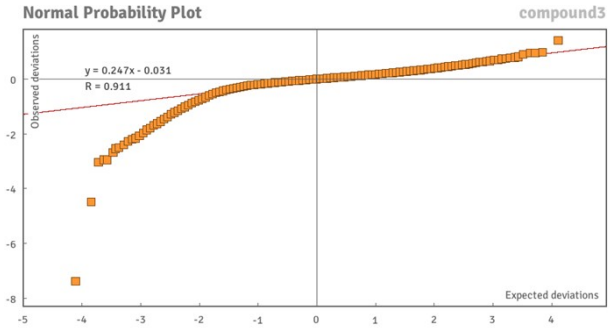
There is a single formula unit in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 2 and Z' is 1. The moiety formula is Mo12 O40 P, 3(C24 H20 P), 2(C8 H9 N O).

Data Plots: Diffraction Data



Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	215666	Unique reflections	25302
Completeness	0.996	Mean I/σ	18.38
hkl_{max} collected	(19, 20, 30)	hkl_{min} collected	(-19, -20, -30)
hkl_{max} used	(19, 20, 30)	hkl_{min} used	(-19, -20, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.36
d_{max} used	9.17	d_{min} used	0.75
Friedel pairs	25199	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0504
R_{sigma}	0.0308	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	34
Multiplicity	(1501, 6780, 12325, 9715, 6904, 6286, 3987, 2449, 537, 20)	Maximum multiplicity	18
Removed systematic absences	0	Filtered off (Shel/OMIT)	0

There are no images if the crystal on the diffractometer, but the inclusion of these images has been requested from the GUI. Please unitck the relevant box if you don't have these images!

Table 10: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **compound3**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Mo11	2668.8(3)	4368.5(3)	1618.5(2)	31.94(9)
Mo8	2549.4(3)	2634.3(3)	4086.8(2)	33.48(10)
Mo7	410.3(3)	2331.6(3)	3361.8(2)	31.95(9)
Mo10	4501.7(3)	2707.4(3)	1637.5(2)	34.19(10)
Mo5	336.9(3)	2469.3(3)	1834.3(2)	34.62(10)
Mo12	2972.4(3)	4393.4(3)	3216.6(2)	34.92(10)
Mo1	2336.1(3)	574.7(3)	3369.5(2)	32.64(9)
Mo4	2480.3(3)	2412.0(3)	946.4(2)	33.36(10)
Mo6	685.4(3)	4250.0(3)	2639.7(2)	36.04(10)
Mo2	4200.2(3)	664.4(3)	2407.9(2)	38.49(11)
Mo3	2041.1(4)	527.6(3)	1859.0(2)	41.09(11)
Mo9	4582.9(3)	2561.1(3)	3257.4(2)	39.69(11)
P1	2485.4(8)	2492.1(7)	2517.1(5)	21.45(19)
O26	2401(2)	3691(2)	993.5(15)	39.8(8)
O18	1106(2)	1264(2)	3361.2(16)	40.0(8)
O20	1335(2)	2688(2)	3887.8(15)	39.5(7)
O32	2629(3)	3799(2)	3972.6(17)	45.1(8)
O27	3101(2)	4543(3)	2421.7(15)	44.3(8)
O24	3746(3)	2372(2)	978.6(16)	43.6(8)
O25	3975(2)	3835(2)	1497.8(16)	40.4(8)

Atom	x	y	z	U_{eq}
O30	4156(2)	3823(2)	3317.6(18)	47.1(9)
O22	4543(3)	1458(2)	3010.1(15)	48.3(9)
O29	1513(2)	4439(3)	1958.6(15)	45.2(8)
O35	1799(3)	-293(2)	1457.1(16)	49.9(9)
O19	2654(2)	1405(2)	3862.7(16)	40.6(8)
O28	1643(2)	4455(3)	3093.2(15)	44.9(8)
O14	1212(3)	2652(2)	1278.5(17)	44.1(8)
O16	75(3)	3621(2)	2048.9(15)	45.3(8)
O8	2944(2)	2850(2)	3046.7(15)	24.1(7)
O17	138(3)	3596(2)	3213.3(15)	44.4(8)
O11	1915(3)	95(3)	2630.8(16)	48.2(9)
O9	3533(3)	193(3)	3100.7(16)	49.7(9)
O21	4476(3)	1473(2)	1869.1(16)	46.8(9)
O38	-35(2)	5177(2)	2636.2(16)	41.6(8)
O23	4740(3)	2865(2)	2415.3(16)	48.0(9)
O33	2134(3)	-233(2)	3832.8(17)	48.7(9)
O6	2864(2)	2833(2)	1946.3(15)	24.2(7)
O12	963(3)	1274(2)	1892.3(17)	47.4(9)
O31	3919(3)	2436(2)	3966.4(18)	49.3(9)
O37	-583(3)	2348(3)	1444.4(17)	54.0(10)
O1	2682(3)	1496(2)	2539.7(15)	25.3(7)
O10	3389(3)	165(3)	1941.6(16)	51.5(9)
O15	-130(3)	2192(2)	2645.0(15)	44.8(8)
O13	2465(3)	1309(2)	1250.3(17)	49.8(9)
O40	2497(3)	2558(3)	4825.8(15)	54.1(10)
O3	1440(2)	2755(2)	2575.9(15)	22.7(6)
O42	5523(3)	2662(3)	1289.7(19)	56.0(10)
O44	3059(3)	5357(2)	3498.2(16)	48.6(9)
O39	-459(3)	2201(3)	3837.4(18)	54.8(10)
O34	5113(3)	-95(2)	2379.4(18)	54.0(10)
O36	2316(3)	2329(3)	227.6(15)	51.4(10)
O43	2721(3)	5325(2)	1291.9(18)	52.2(10)
O41	5653(3)	2551(3)	3493.9(18)	51.0(9)
P4	936.1(10)	7423.1(9)	4012.4(6)	38.1(3)
C51	145(4)	8369(3)	4209(2)	42.0(12)
C57	1233(4)	7426(3)	3236(2)	39.5(11)
C56	88(4)	9113(4)	3866(3)	54.4(15)
C63	378(4)	6481(3)	4165(2)	41.0(12)
C45	1966(4)	7399(3)	4429(2)	44.1(12)
C58	1755(5)	8040(4)	2993(3)	55.7(16)
C65	477(5)	4944(4)	4297(3)	57.1(17)
C64	903(4)	5697(4)	4270(2)	46.7(13)
C52	-354(4)	8359(4)	4743(3)	58.6(16)
C68	-571(5)	6526(4)	4093(3)	62.1(17)
C62	956(4)	6802(4)	2876(2)	50.9(14)
C66	-452(6)	4992(4)	4233(3)	65.0(19)
C61	1172(5)	6803(5)	2278(3)	67.6(19)
C59	1967(5)	8033(4)	2396(3)	69(2)
C50	2829(4)	7139(4)	4171(3)	58.3(16)
C67	-981(5)	5775(5)	4132(3)	70.0(19)
C46	1906(5)	7625(5)	5018(3)	68.4(19)
C53	-902(5)	9096(5)	4926(4)	73(2)
C55	-471(5)	9856(4)	4060(4)	72(2)
C54	-958(5)	9840(5)	4587(4)	83(3)
C48	3542(6)	7356(6)	5074(4)	84(2)
C49	3614(5)	7119(5)	4502(4)	72(2)
C60	1659(6)	7421(5)	2040(3)	75(2)
C47	2705(6)	7597(6)	5339(3)	88(3)
P2	7618.5(10)	5831.4(10)	1512.5(7)	47.6(3)
C19	7517(4)	4940(4)	2013(3)	48.9(13)
C6	9252(4)	4857(4)	1144(2)	48.6(14)
C13	6668(4)	5909(4)	1027(3)	50.8(14)
C7	7640(4)	6827(4)	1903(3)	51.6(14)

Atom	x	y	z	U_{eq}
C5	10113(4)	4754(5)	878(3)	59.2(17)
C24	7873(4)	4930(4)	2577(3)	55.8(15)
C15	6017(5)	6032(5)	70(3)	67.8(19)
C1	8701(4)	5642(4)	1109(2)	45.9(13)
C4	10433(5)	5412(5)	570(3)	66.2(18)
C14	6777(4)	5971(4)	421(3)	56.9(16)
C16	5156(5)	6026(5)	313(3)	71(2)
C8	6889(5)	7471(4)	1918(3)	62.5(17)
C12	8440(5)	6964(4)	2187(3)	71(2)
C20	7145(6)	4216(5)	1826(3)	76(2)
C23	7869(5)	4196(5)	2935(3)	71(2)
C2	9008(5)	6321(4)	774(3)	68.0(19)
C9	6943(6)	8221(5)	2220(4)	80(2)
C3	9878(5)	6190(5)	513(4)	78(2)
C18	5784(5)	5904(6)	1267(3)	86(3)
C10	7717(6)	8345(5)	2505(4)	82(2)
C22	7486(6)	3503(5)	2744(4)	81(2)
C11	8473(6)	7713(5)	2487(4)	81(2)
C17	5034(5)	5965(7)	907(3)	89(3)
C21	7122(7)	3508(5)	2194(4)	89(3)
P3	7575.1(9)	401.4(9)	820.8(6)	36.2(3)
C37	6529(4)	-65(4)	734(2)	40.3(12)
C39	7723(4)	582(3)	1591(2)	38.5(11)
C31	7498(3)	1418(4)	428(2)	39.2(11)
C25	8533(4)	-338(4)	538(2)	43.1(12)
C102	5679(4)	462(4)	766(2)	47.7(13)
C40	6957(4)	722(4)	1967(2)	52.4(14)
C42	7935(5)	890(5)	2776(3)	64.0(18)
C38	6561(4)	-947(4)	684(3)	54.1(15)
C32	7741(4)	2147(4)	697(3)	46.9(13)
C26	8766(4)	-324(4)	-61(3)	55.1(15)
C101	4872(4)	90(5)	787(3)	59.4(17)
C43	8705(5)	740(4)	2408(3)	61.2(18)
C44	8605(4)	598(4)	1813(2)	52.3(15)
C41	7068(5)	880(5)	2561(3)	66.0(18)
C33	7708(5)	2916(4)	375(3)	61.2(17)
C34	7424(5)	2961(5)	-195(3)	73(2)
C35	7173(5)	2248(6)	-461(3)	79(2)
C27	9480(5)	-916(5)	-278(4)	71(2)
C100	4915(5)	-794(6)	764(3)	71(2)
C28	9956(5)	-1495(5)	84(4)	82(3)
C99	5733(5)	-1302(5)	699(3)	72(2)
C36	7208(4)	1474(5)	-155(3)	59.9(17)
C30	9010(5)	-949(4)	902(3)	63.6(17)
C29	9736(6)	-1522(5)	678(4)	86(2)
O47	3971(5)	7688(5)	1630(3)	113(2)
N3	4493(5)	7222(4)	2525(3)	80.0(18)
C97	4371(5)	7795(5)	2078(4)	75(2)
C85	5035(15)	7368(12)	3002(8)	68(5)
C98	4123(7)	6405(6)	2501(4)	105(3)
C90	4959(15)	8157(13)	3257(8)	77(5)
C86	5625(18)	6590(14)	3201(10)	108(7)
C88	6170(20)	7583(16)	3886(11)	108(7)
C89	5565(19)	8287(13)	3697(9)	96(6)
C87	6269(18)	6796(16)	3595(11)	122(7)
O45	6623(12)	623(11)	3937(6)	137(6)
N1	5824(10)	273(10)	4751(6)	90(4)
C69	4980(20)	138(12)	5046(11)	55(4)
C71	3357(12)	497(12)	5161(8)	81(5)
C75	5870(30)	480(30)	4170(20)	82(13)
C74	4998(12)	-446(10)	5515(7)	77(4)
C70	4169(12)	606(11)	4880(7)	89(5)
C72	3344(13)	-97(13)	5620(10)	100(6)

Atom	x	y	z	U_{eq}
C76	6636(14)	185(17)	5098(10)	122(7)
C73	4140(40)	-590(40)	5760(30)	110(18)
O46	2625(8)	5227(9)	5432(6)	109(4)
N2	4191(7)	5145(7)	5359(5)	57(2)
C84	4250(30)	5300(50)	5981(18)	79(8)
C78	5741(10)	5452(10)	5179(6)	68(4)
C79	6535(15)	5382(14)	4824(10)	91(7)
C82	5060(10)	4612(9)	4478(6)	64(3)
C80	6593(14)	4912(13)	4304(8)	99(6)
C81	5860(40)	4560(40)	4116(19)	90(14)
C83	3348(13)	5132(12)	5141(10)	73(5)
C77	5000(50)	5060(40)	5000(40)	50(4)
C91	4934(13)	7461(11)	3049(8)	84(6)
C96	4570(16)	8219(10)	3335(9)	101(7)
C95	4990(20)	8477(11)	3834(8)	124(8)
C94	5771(18)	7977(16)	4048(8)	134(8)
C93	6135(12)	7219(17)	3762(9)	133(9)
C92	5717(12)	6961(13)	3262(8)	106(7)
O7	2315(10)	3521(9)	2457(7)	29(3)
O2	2025(12)	2173(10)	1949(6)	32(4)
O5	3531(10)	2245(10)	2418(7)	34(4)
O4	2106(11)	2192(10)	3057(7)	33(4)

Table 11: Anisotropic Displacement Parameters ($\times 10^4$) for **compound3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mo11	39.7(2)	27.8(2)	28.33(19)	5.90(15)	1.81(16)	-6.11(16)
Mo8	46.5(2)	33.1(2)	22.18(18)	0.91(15)	-2.92(16)	-9.97(18)
Mo7	32.8(2)	34.6(2)	27.99(19)	3.90(16)	5.04(16)	-4.85(17)
Mo10	30.3(2)	38.4(2)	33.2(2)	4.60(17)	4.40(16)	-4.28(17)
Mo5	30.0(2)	35.6(2)	40.0(2)	-3.59(17)	-11.16(17)	-8.16(17)
Mo12	37.6(2)	26.4(2)	42.4(2)	-9.90(17)	-6.67(18)	-7.73(17)
Mo1	43.2(2)	27.7(2)	27.69(19)	5.22(15)	0.05(17)	-7.75(17)
Mo4	43.5(2)	35.5(2)	21.42(18)	0.57(15)	1.42(16)	-6.92(18)
Mo6	35.2(2)	30.3(2)	39.8(2)	-3.78(17)	-5.77(18)	7.78(17)
Mo2	37.5(2)	30.0(2)	44.3(2)	-2.96(18)	0.43(19)	8.97(17)
Mo3	57.6(3)	27.9(2)	39.5(2)	-11.29(17)	-2.6(2)	-10.43(19)
Mo9	30.7(2)	42.7(2)	45.9(3)	0.90(19)	-15.03(19)	-2.88(18)
P1	24.3(5)	19.4(4)	20.8(4)	-1.7(4)	-2.6(4)	-3.0(4)
O26	41.0(19)	35.7(17)	42.3(18)	-1.5(14)	-7.8(15)	-1.3(14)
O18	42.8(18)	32.4(17)	46(2)	-2.3(14)	-10.8(14)	-4.4(14)
O20	42.9(18)	31.2(17)	44.3(18)	-5.7(14)	-7.2(14)	-2.3(14)
O32	46(2)	33.3(17)	55(2)	2.6(15)	6.0(16)	-3.6(14)
O27	35.4(18)	61(2)	37.7(17)	-6.0(15)	-3.7(13)	-7.7(17)
O24	47(2)	39.5(19)	43.7(19)	-7.5(15)	-3.1(15)	-1.5(15)
O25	35.7(18)	38.7(18)	47(2)	-1.5(14)	-7.2(14)	-4.1(14)
O30	37.3(19)	38.6(18)	66(2)	8.4(16)	2.6(16)	-8.0(14)
O22	67(2)	43.2(19)	34.7(17)	5.6(14)	-12.2(17)	-7.4(16)
O29	36.0(18)	65(2)	34.1(17)	-4.0(16)	-4.6(14)	-4.2(16)
O35	80(3)	30.4(18)	41.3(19)	-8.2(15)	-8.9(19)	-12.9(17)
O19	44.1(19)	31.3(16)	46.0(19)	-1.5(14)	-13.8(16)	-0.7(14)
O28	37.6(18)	63(2)	33.9(17)	-10.0(16)	-0.7(14)	-5.0(15)
O14	42.9(19)	34.1(18)	54(2)	4.8(15)	6.8(16)	-2.7(14)
O16	68(2)	33.2(17)	34.3(17)	4.7(13)	-15.2(16)	-5.2(16)
O8	28.9(17)	22.6(16)	21.5(14)	-1.0(12)	-4.6(12)	-4.9(13)
O17	64(2)	33.3(17)	35.3(17)	-3.9(13)	-7.6(16)	-4.5(15)
O11	52(2)	56(2)	38.7(18)	-6.6(16)	-2.8(15)	-13.6(18)
O9	48(2)	61(2)	39.6(19)	-0.2(17)	-0.2(15)	-3.2(17)
O21	68(2)	35.1(18)	37.3(18)	-0.1(14)	-6.3(16)	-6.6(16)
O38	37.0(18)	30.0(17)	56(2)	1.5(15)	-1.3(16)	3.4(14)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O23	64(2)	40.9(19)	40.6(18)	3.4(14)	-9.6(15)	-12.1(18)
O33	60(2)	33.1(18)	54(2)	12.6(16)	-6.9(18)	-12.8(16)
O6	28.6(17)	23.6(16)	20.3(14)	2.2(12)	-0.8(12)	-3.2(13)
O12	51(2)	32.2(17)	60(2)	4.7(15)	9.0(16)	-9.8(15)
O31	46(2)	42(2)	57(2)	9.5(17)	2.9(16)	0.3(16)
O37	43(2)	78(3)	46(2)	5.5(19)	-17.2(17)	-24.9(19)
O1	32.2(18)	18.3(12)	25.2(16)	-1.3(12)	-1.2(14)	-2.1(12)
O10	56(2)	61(2)	37.9(19)	-11.9(17)	4.6(16)	-7.1(18)
O15	63(2)	36.6(18)	36.4(17)	1.0(14)	-8.4(15)	-11.7(17)
O13	57(2)	32.4(18)	57(2)	4.3(16)	15.2(18)	0.6(15)
O40	70(3)	63(3)	28.3(18)	-4.9(16)	-9.3(16)	-4(2)
O3	24.4(13)	21.2(16)	22.6(16)	-0.1(13)	-2.0(12)	-3.1(12)
O42	40(2)	62(3)	66(3)	-7(2)	17.8(18)	-9.2(17)
O44	75(3)	32.8(18)	41(2)	-7.8(15)	-0.8(18)	-19.9(17)
O39	46(2)	65(3)	54(2)	-5.2(19)	18.7(18)	-13.2(19)
O34	53(2)	41(2)	61(2)	6.7(17)	9.9(18)	16.7(18)
O36	68(3)	58(2)	27.2(17)	-7.4(15)	-8.1(16)	-3(2)
O43	61(2)	32.8(18)	65(2)	18.6(17)	-10(2)	-13.9(16)
O41	36.4(19)	60(2)	57(2)	0.6(19)	-18.0(17)	-5.8(17)
P4	44.8(8)	35.3(7)	34.8(6)	-3.1(5)	5.5(5)	-9.1(6)
C51	40(3)	39(3)	46(3)	-4(2)	2(2)	-5(2)
C57	50(3)	34(3)	35(3)	-3(2)	4(2)	-10(2)
C56	44(3)	51(3)	67(4)	6(3)	0(3)	-4(3)
C63	50(3)	42(3)	33(2)	-1(2)	9(2)	-16(2)
C45	48(3)	38(3)	46(3)	-6(2)	1(2)	-6(2)
C58	75(4)	37(3)	57(4)	-8(3)	22(3)	-20(3)
C65	84(5)	40(3)	46(3)	-4(2)	21(3)	-9(3)
C64	53(3)	44(3)	42(3)	-2(2)	15(2)	-8(3)
C52	57(4)	64(4)	52(4)	-9(3)	13(3)	-3(3)
C68	58(4)	54(4)	76(4)	10(3)	2(3)	-15(3)
C62	68(4)	50(3)	40(3)	-5(2)	6(3)	-26(3)
C66	95(6)	57(4)	50(4)	-10(3)	22(3)	-42(4)
C61	90(5)	77(5)	41(3)	-15(3)	8(3)	-31(4)
C59	103(6)	40(3)	62(4)	7(3)	33(4)	-12(3)
C50	55(4)	62(4)	56(4)	-14(3)	-1(3)	-1(3)
C67	63(4)	73(5)	80(5)	7(4)	3(4)	-33(4)
C46	65(4)	98(6)	41(3)	-13(3)	4(3)	-5(4)
C53	61(4)	74(5)	81(5)	-16(4)	23(4)	1(4)
C55	55(4)	46(4)	114(6)	9(4)	0(4)	-1(3)
C54	56(4)	56(4)	134(8)	-24(5)	12(5)	8(3)
C48	74(5)	90(6)	88(6)	-8(5)	-29(5)	-2(4)
C49	50(4)	85(5)	81(5)	-16(4)	-4(4)	-3(4)
C60	117(7)	64(4)	41(3)	1(3)	21(4)	-14(4)
C47	87(6)	125(7)	50(4)	-18(4)	-20(4)	-4(5)
P2	39.3(8)	52.8(9)	47.9(8)	2.2(7)	4.3(6)	2.8(6)
C19	46(3)	53(3)	47(3)	4(3)	4(2)	-3(3)
C6	46(3)	54(3)	42(3)	14(3)	0(2)	4(3)
C13	35(3)	63(4)	52(3)	0(3)	3(2)	0(3)
C7	48(3)	50(3)	53(3)	3(3)	2(3)	5(3)
C5	50(4)	74(4)	45(3)	13(3)	-1(3)	22(3)
C24	43(3)	66(4)	60(4)	5(3)	-8(3)	-10(3)
C15	64(4)	91(5)	48(4)	19(3)	-1(3)	-13(4)
C1	36(3)	51(3)	48(3)	2(2)	3(2)	1(2)
C4	45(4)	93(5)	59(4)	-8(4)	8(3)	-3(3)
C14	49(3)	70(4)	50(3)	19(3)	8(3)	-9(3)
C16	51(4)	97(6)	65(4)	-1(4)	-11(3)	-5(4)
C8	48(4)	57(4)	76(4)	5(3)	3(3)	12(3)
C12	65(4)	50(4)	93(5)	-5(4)	-18(4)	12(3)
C20	103(6)	78(5)	54(4)	2(4)	-8(4)	-30(5)
C23	59(4)	93(6)	60(4)	20(4)	-11(3)	-12(4)
C2	66(4)	46(4)	88(5)	4(3)	20(4)	1(3)
C9	72(5)	55(4)	103(6)	-2(4)	17(5)	21(4)
C3	76(5)	61(4)	99(6)	-4(4)	36(4)	-22(4)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C18	48(4)	164(9)	46(4)	-5(4)	8(3)	-15(5)
C10	97(6)	54(4)	95(6)	-10(4)	1(5)	-4(4)
C22	84(6)	81(5)	81(5)	27(4)	-2(4)	-23(4)
C11	82(5)	56(4)	106(6)	-7(4)	-31(5)	-3(4)
C17	42(4)	161(9)	65(5)	-6(5)	4(3)	-17(5)
C21	121(7)	73(5)	81(6)	5(4)	3(5)	-47(5)
P3	32.6(6)	47.2(7)	30.6(6)	-4.4(5)	2.2(5)	-11.9(6)
C37	39(3)	55(3)	30(2)	-9(2)	4(2)	-18(2)
C39	41(3)	45(3)	31(2)	0(2)	-4(2)	-11(2)
C31	29(2)	52(3)	38(3)	3(2)	-1(2)	-10(2)
C25	33(3)	49(3)	49(3)	-8(2)	5(2)	-12(2)
C102	39(3)	63(4)	42(3)	-12(3)	4(2)	-10(3)
C40	50(3)	73(4)	34(3)	-7(3)	1(2)	-7(3)
C42	89(5)	74(5)	34(3)	-3(3)	-12(3)	-30(4)
C38	54(4)	54(4)	58(4)	-3(3)	-10(3)	-15(3)
C32	39(3)	55(3)	48(3)	1(3)	-4(2)	-8(2)
C26	53(4)	64(4)	50(3)	-17(3)	12(3)	-13(3)
C101	36(3)	104(6)	41(3)	-4(3)	-2(2)	-19(3)
C43	75(5)	75(4)	42(3)	7(3)	-18(3)	-39(4)
C44	52(3)	69(4)	42(3)	8(3)	-6(3)	-30(3)
C41	80(5)	82(5)	35(3)	-10(3)	6(3)	-11(4)
C33	56(4)	50(4)	77(5)	7(3)	-3(3)	-9(3)
C34	60(4)	78(5)	79(5)	35(4)	-7(4)	-4(4)
C35	69(5)	118(7)	50(4)	32(4)	-15(3)	-17(5)
C27	67(5)	73(5)	78(5)	-30(4)	35(4)	-28(4)
C100	55(4)	106(6)	63(4)	22(4)	-19(3)	-45(4)
C28	65(5)	55(4)	126(7)	-25(5)	41(5)	-12(4)
C99	77(5)	63(4)	86(5)	10(4)	-30(4)	-40(4)
C36	58(4)	83(5)	42(3)	8(3)	-12(3)	-19(3)
C30	62(4)	58(4)	67(4)	1(3)	9(3)	2(3)
C29	71(5)	64(5)	116(7)	-1(5)	13(5)	10(4)
O47	128(6)	153(6)	70(4)	-8(4)	-7(4)	-55(5)
N3	94(5)	68(4)	80(4)	5(3)	23(4)	-25(3)
C97	72(5)	82(5)	74(5)	7(4)	2(4)	-20(4)
C85	72(10)	67(9)	64(9)	11(8)	11(8)	-12(9)
C98	142(8)	83(6)	98(6)	-18(5)	57(6)	-54(6)
C90	78(11)	78(10)	77(10)	13(8)	-14(8)	-18(9)
C86	128(14)	89(12)	103(12)	19(11)	-4(11)	4(11)
C88	130(14)	96(13)	93(12)	-12(10)	-43(11)	14(11)
C89	104(13)	95(11)	91(11)	-1(9)	-31(10)	-12(10)
C87	153(15)	103(13)	105(13)	0(11)	-44(12)	9(12)
O45	134(13)	164(15)	101(10)	54(10)	46(9)	14(11)
N1	75(8)	117(10)	69(7)	43(7)	-16(6)	16(7)
C69	56(5)	60(8)	48(6)	11(6)	-12(4)	-1(6)
C71	57(9)	93(12)	91(12)	35(10)	-27(9)	-5(9)
C75	69(18)	110(30)	56(13)	34(15)	3(12)	27(18)
C74	85(11)	67(9)	73(10)	30(8)	-15(9)	18(8)
C70	84(12)	101(13)	83(11)	60(10)	-36(9)	-10(10)
C72	71(11)	105(14)	122(16)	49(13)	-12(11)	-8(10)
C76	76(11)	171(16)	108(13)	65(13)	-8(10)	16(12)
C73	150(40)	80(20)	110(40)	50(20)	-10(30)	-40(20)
O46	58(6)	141(11)	134(11)	-3(9)	5(6)	-40(7)
N2	57(5)	57(6)	61(6)	2(5)	-10(4)	-23(5)
C84	81(15)	100(20)	60(8)	-9(10)	-4(7)	-26(13)
C78	70(7)	90(10)	51(7)	-14(6)	-7(5)	-38(7)
C79	81(10)	117(16)	87(11)	-40(12)	13(8)	-56(12)
C82	62(7)	70(8)	67(7)	-16(6)	-17(5)	-28(6)
C80	91(11)	127(15)	89(11)	-45(10)	22(9)	-57(11)
C81	95(14)	100(30)	81(19)	-50(20)	13(13)	-43(16)
C83	57(6)	87(12)	79(10)	3(10)	-15(5)	-27(8)
C77	52(4)	49(11)	50(4)	1(8)	-14(3)	-12(7)
C91	74(10)	76(10)	105(12)	24(10)	-5(10)	-26(9)
C96	101(14)	82(11)	131(14)	11(10)	-43(11)	-41(10)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C95	125(16)	108(13)	146(15)	8(11)	-62(13)	-27(11)
C94	132(16)	129(16)	142(16)	29(13)	-62(13)	-14(13)
C93	121(15)	122(17)	150(17)	20(15)	-22(14)	3(14)
C92	88(12)	97(13)	127(14)	58(11)	-4(11)	2(10)
O7	28(8)	23(7)	37(8)	9(6)	-9(6)	-5(6)
O2	47(10)	30(8)	21(7)	-1(6)	-10(7)	-3(7)
O5	23(8)	29(8)	49(10)	1(7)	-6(7)	-4(6)
O4	42(9)	35(9)	25(8)	1(6)	-3(7)	-13(7)

Table 12: Bond Lengths in Å for **compound3**.

Atom	Atom	Length/Å
Mo11	O26	1.858(3)
Mo11	O27	1.975(3)
Mo11	O25	1.992(3)
Mo11	O29	1.825(4)
Mo11	O6	2.473(3)
Mo11	O43	1.660(3)
Mo11	O7	2.373(14)
Mo8	O20	1.835(3)
Mo8	O32	1.845(3)
Mo8	O19	1.972(3)
Mo8	O8	2.433(3)
Mo8	O31	1.995(4)
Mo8	O40	1.673(4)
Mo8	O4	2.565(15)
Mo7	O18	1.830(3)
Mo7	O20	1.965(3)
Mo7	O17	1.980(3)
Mo7	O15	1.852(3)
Mo7	O3	2.432(3)
Mo7	O39	1.670(4)
Mo7	O4	2.535(16)
Mo10	O24	1.997(4)
Mo10	O25	1.847(3)
Mo10	O21	1.987(4)
Mo10	O23	1.830(4)
Mo10	O6	2.457(4)
Mo10	O42	1.659(4)
Mo10	O5	2.392(16)
Mo5	O14	1.811(4)
Mo5	O16	1.852(4)
Mo5	O12	1.966(4)
Mo5	O37	1.662(4)
Mo5	O15	1.997(4)
Mo5	O3	2.446(3)
Mo5	O2	2.469(17)
Mo12	O32	2.011(4)
Mo12	O27	1.816(4)
Mo12	O30	1.856(4)
Mo12	O28	1.959(4)
Mo12	O8	2.444(3)
Mo12	O44	1.660(3)
Mo12	O7	2.497(15)
Mo1	O18	1.968(3)
Mo1	O19	1.835(3)
Mo1	O11	1.987(4)
Mo1	O9	1.859(4)
Mo1	O33	1.673(3)
Mo1	O1	2.423(4)
Mo1	O4	2.585(16)
Mo4	O26	1.982(3)

Atom	Atom	Length/Å
Mo4	O24	1.845(4)
Mo4	O14	1.970(4)
Mo4	O6	2.465(3)
Mo4	O13	1.840(4)
Mo4	O36	1.660(3)
Mo4	O2	2.380(15)
Mo6	O29	1.971(4)
Mo6	O28	1.824(4)
Mo6	O16	1.970(4)
Mo6	O17	1.861(4)
Mo6	O38	1.670(3)
Mo6	O3	2.444(3)
Mo6	O7	2.524(15)
Mo2	O22	1.972(4)
Mo2	O9	1.999(4)
Mo2	O21	1.811(4)
Mo2	O1	2.429(4)
Mo2	O10	1.862(4)
Mo2	O34	1.662(4)
Mo2	O5	2.525(15)
Mo3	O35	1.661(3)
Mo3	O11	1.872(4)
Mo3	O12	1.830(4)
Mo3	O1	2.460(4)
Mo3	O10	1.990(4)
Mo3	O13	1.961(4)
Mo3	O2	2.569(15)
Mo9	O30	1.986(4)
Mo9	O22	1.822(4)
Mo9	O8	2.437(4)
Mo9	O23	1.968(4)
Mo9	O31	1.870(4)
Mo9	O41	1.666(4)
Mo9	O5	2.570(16)
P1	O8	1.537(3)
P1	O6	1.504(3)
P1	O1	1.539(4)
P1	O3	1.530(4)
P1	O7	1.592(14)
P1	O2	1.585(14)
P1	O5	1.536(15)
P1	O4	1.421(15)
P4	C51	1.800(5)
P4	C57	1.794(5)
P4	C63	1.793(5)
P4	C45	1.795(6)
C51	C56	1.378(8)
C51	C52	1.394(8)
C57	C58	1.395(7)
C57	C62	1.386(7)

Atom	Atom	Length/Å
C56	C55	1.394(9)
C63	C64	1.374(8)
C63	C68	1.394(8)
C45	C50	1.386(8)
C45	C46	1.381(8)
C58	C59	1.377(8)
C65	C64	1.396(8)
C65	C66	1.362(10)
C52	C53	1.372(9)
C68	C67	1.380(9)
C62	C61	1.379(8)
C66	C67	1.375(10)
C61	C60	1.364(9)
C59	C60	1.384(10)
C50	C49	1.386(9)
C46	C47	1.389(10)
C53	C54	1.372(11)
C55	C54	1.371(11)
C48	C49	1.347(10)
C48	C47	1.357(11)
P2	C19	1.794(6)
P2	C13	1.786(6)
P2	C7	1.800(6)
P2	C1	1.795(5)
C19	C24	1.390(8)
C19	C20	1.390(9)
C6	C5	1.369(8)
C6	C1	1.374(7)
C13	C14	1.378(8)
C13	C18	1.386(8)
C7	C8	1.385(8)
C7	C12	1.393(9)
C5	C4	1.354(10)
C24	C23	1.389(9)
C15	C14	1.377(9)
C15	C16	1.358(9)
C1	C2	1.402(8)
C4	C3	1.371(10)
C16	C17	1.354(10)
C8	C9	1.375(10)
C12	C11	1.366(10)
C20	C21	1.373(10)
C23	C22	1.361(11)
C2	C3	1.378(9)
C9	C10	1.355(11)
C18	C17	1.377(10)
C10	C11	1.379(10)
C22	C21	1.365(11)
P3	C37	1.793(5)
P3	C39	1.793(5)
P3	C31	1.793(5)
P3	C25	1.800(5)
C37	C102	1.395(8)
C37	C38	1.374(8)
C39	C40	1.380(7)
C39	C44	1.399(7)
C31	C32	1.388(8)
C31	C36	1.394(7)
C25	C26	1.387(8)
C25	C30	1.378(9)
C102	C101	1.380(8)
C40	C41	1.388(8)
C42	C43	1.376(10)
C42	C41	1.372(10)
C38	C99	1.394(9)
C32	C33	1.385(8)
C26	C27	1.382(9)
C101	C100	1.370(10)
C43	C44	1.383(8)
C33	C34	1.364(10)
C34	C35	1.367(11)
C35	C36	1.375(10)
C27	C28	1.346(11)
C100	C99	1.349(11)
C28	C29	1.372(12)
C30	C29	1.384(9)
O47	C97	1.210(9)
N3	C97	1.336(9)
N3	C85	1.395(14)
N3	C98	1.447(9)
N3	C91	1.442(12)
C85	C90	1.354(14)
C85	C86	1.464(11)
C90	C89	1.387(15)
C86	C87	1.386(17)
C88	C89	1.383(16)
C88	C87	1.388(16)
O45	C75	1.25(5)
N1	C69	1.42(3)
N1	C75	1.35(5)
N1	C76	1.43(2)
C69	C74	1.38(3)
C69	C70	1.37(3)
C71	C70	1.36(2)
C71	C72	1.38(2)
C74	C73	1.40(6)
C72	C73	1.35(5)
O46	C83	1.22(2)
N2	C84	1.44(4)
N2	C83	1.34(2)
N2	C77	1.41(8)
C78	C79	1.38(2)
C78	C77	1.39(7)
C79	C80	1.39(2)
C82	C81	1.40(5)
C82	C77	1.37(7)
C80	C81	1.34(5)
C91	C96	1.3900
C91	C92	1.3900
C96	C95	1.3900
C95	C94	1.3900
C94	C93	1.3900
C93	C92	1.3900

Table 13: Bond Angles in ° for **compound3**.

Atom	Atom	Atom	Angle/°
O26	Mo11	O27	153.62(16)
O26	Mo11	O25	86.29(15)
O26	Mo11	O6	71.36(13)
O26	Mo11	O7	102.4(4)
O27	Mo11	O25	81.87(15)
O27	Mo11	O6	82.40(14)
O27	Mo11	O7	56.3(4)
O25	Mo11	O6	69.40(13)
O25	Mo11	O7	97.2(4)
O29	Mo11	O26	94.51(16)
O29	Mo11	O27	86.23(15)
O29	Mo11	O25	153.98(16)
O29	Mo11	O6	86.18(15)
O29	Mo11	O7	57.2(4)
O43	Mo11	O26	102.36(18)
O43	Mo11	O27	102.84(18)
O43	Mo11	O25	99.80(18)
O43	Mo11	O29	105.39(19)
O43	Mo11	O6	167.46(17)
O43	Mo11	O7	150.7(4)
O20	Mo8	O32	96.17(16)
O20	Mo8	O19	85.47(14)
O20	Mo8	O8	88.70(14)
O20	Mo8	O31	157.04(16)
O20	Mo8	O4	59.0(4)
O32	Mo8	O19	155.89(16)
O32	Mo8	O8	72.62(14)
O32	Mo8	O31	87.00(16)
O32	Mo8	O4	101.7(4)
O19	Mo8	O8	83.39(13)
O19	Mo8	O31	82.64(15)
O19	Mo8	O4	58.7(4)
O31	Mo8	O8	70.49(14)
O31	Mo8	O4	98.1(4)
O40	Mo8	O20	102.87(19)
O40	Mo8	O32	101.56(19)
O40	Mo8	O19	101.50(18)
O40	Mo8	O8	167.68(17)
O40	Mo8	O31	98.72(19)
O40	Mo8	O4	151.9(4)
O18	Mo7	O20	86.30(14)
O18	Mo7	O17	156.50(16)
O18	Mo7	O15	95.08(16)
O18	Mo7	O3	87.53(14)
O18	Mo7	O4	60.2(4)
O20	Mo7	O17	82.86(14)
O20	Mo7	O3	84.11(13)
O20	Mo7	O4	58.6(4)
O17	Mo7	O3	70.69(14)
O17	Mo7	O4	96.5(4)
O15	Mo7	O20	155.96(16)
O15	Mo7	O17	86.69(15)
O15	Mo7	O3	72.00(14)
O15	Mo7	O4	101.5(4)
O39	Mo7	O18	103.25(19)
O39	Mo7	O20	101.85(18)
O39	Mo7	O17	99.36(19)
O39	Mo7	O15	101.17(19)
O39	Mo7	O3	167.89(17)
O39	Mo7	O4	152.9(4)
O24	Mo10	O6	69.59(13)
O24	Mo10	O5	95.7(4)
O25	Mo10	O24	86.83(15)
O25	Mo10	O21	154.32(16)
O25	Mo10	O6	71.82(14)
O25	Mo10	O5	102.5(4)
O21	Mo10	O24	81.67(15)
O21	Mo10	O6	82.65(14)
O21	Mo10	O5	56.4(4)
O23	Mo10	O24	154.12(17)
O23	Mo10	O25	95.60(16)
O23	Mo10	O21	85.35(15)
O23	Mo10	O6	86.65(15)
O23	Mo10	O5	58.5(4)
O42	Mo10	O24	99.79(19)
O42	Mo10	O25	103.02(19)
O42	Mo10	O21	101.52(19)
O42	Mo10	O23	104.7(2)
O42	Mo10	O6	168.11(18)
O42	Mo10	O5	150.7(4)
O14	Mo5	O16	95.24(17)
O14	Mo5	O12	86.62(15)
O14	Mo5	O15	155.17(17)
O14	Mo5	O3	87.19(15)
O14	Mo5	O2	53.8(4)
O16	Mo5	O12	155.32(16)
O16	Mo5	O15	85.98(15)
O16	Mo5	O3	71.84(14)
O16	Mo5	O2	102.6(4)
O12	Mo5	O15	82.36(15)
O12	Mo5	O3	83.70(14)
O12	Mo5	O2	59.0(4)
O37	Mo5	O14	104.01(19)
O37	Mo5	O16	101.2(2)
O37	Mo5	O12	102.20(19)
O37	Mo5	O15	100.04(18)
O37	Mo5	O3	167.51(17)
O37	Mo5	O2	148.7(4)
O15	Mo5	O3	69.58(13)
O15	Mo5	O2	101.6(4)
O32	Mo12	O8	69.92(13)
O32	Mo12	O7	101.8(4)
O27	Mo12	O32	156.49(16)
O27	Mo12	O30	95.52(17)
O27	Mo12	O28	86.78(15)
O27	Mo12	O8	88.27(15)
O27	Mo12	O7	55.0(4)
O30	Mo12	O32	86.20(16)
O30	Mo12	O28	154.50(16)
O30	Mo12	O8	71.94(14)
O30	Mo12	O7	104.0(4)
O28	Mo12	O32	81.99(15)
O28	Mo12	O8	82.78(14)
O28	Mo12	O7	57.1(4)
O44	Mo12	O32	97.67(17)
O44	Mo12	O27	104.92(18)
O44	Mo12	O30	101.39(19)
O44	Mo12	O28	102.52(19)
O44	Mo12	O8	165.93(15)
O44	Mo12	O7	148.8(3)
O18	Mo1	O11	82.85(15)
O18	Mo1	O1	84.43(14)
O18	Mo1	O4	58.0(4)
O19	Mo1	O18	86.01(15)
O19	Mo1	O11	157.01(16)
O19	Mo1	O9	95.84(17)

Atom	Atom	Atom	Angle/°
O19	Mo1	O1	88.13(14)
O19	Mo1	O4	59.4(3)
O11	Mo1	O1	70.85(14)
O11	Mo1	O4	97.8(4)
O9	Mo1	O18	156.69(16)
O9	Mo1	O11	86.80(16)
O9	Mo1	O1	72.43(15)
O9	Mo1	O4	103.2(4)
O33	Mo1	O18	100.81(17)
O33	Mo1	O19	103.52(18)
O33	Mo1	O11	98.30(18)
O33	Mo1	O9	101.33(19)
O33	Mo1	O1	167.45(16)
O33	Mo1	O4	151.3(4)
O26	Mo4	O6	69.80(13)
O26	Mo4	O2	96.4(4)
O24	Mo4	O26	87.46(15)
O24	Mo4	O14	153.45(16)
O24	Mo4	O6	71.57(14)
O24	Mo4	O2	103.3(4)
O14	Mo4	O26	81.72(15)
O14	Mo4	O6	81.94(14)
O14	Mo4	O2	54.5(4)
O13	Mo4	O26	154.81(16)
O13	Mo4	O24	94.48(17)
O13	Mo4	O14	85.60(16)
O13	Mo4	O6	86.96(15)
O13	Mo4	O2	58.7(4)
O36	Mo4	O26	98.99(17)
O36	Mo4	O24	102.70(19)
O36	Mo4	O14	102.89(19)
O36	Mo4	O6	167.27(17)
O36	Mo4	O13	105.03(19)
O36	Mo4	O2	150.3(4)
O29	Mo6	O3	83.47(14)
O29	Mo6	O7	53.0(3)
O28	Mo6	O29	85.50(15)
O28	Mo6	O16	154.92(16)
O28	Mo6	O17	95.36(16)
O28	Mo6	O3	86.69(15)
O28	Mo6	O7	57.5(4)
O16	Mo6	O29	82.42(16)
O16	Mo6	O3	70.18(13)
O16	Mo6	O7	97.9(4)
O17	Mo6	O29	155.52(16)
O17	Mo6	O16	86.90(15)
O17	Mo6	O3	72.18(14)
O17	Mo6	O7	107.4(3)
O38	Mo6	O29	101.13(17)
O38	Mo6	O28	105.33(18)
O38	Mo6	O16	98.54(17)
O38	Mo6	O17	102.20(17)
O38	Mo6	O3	167.34(15)
O38	Mo6	O7	146.8(3)
O22	Mo2	O9	82.24(16)
O22	Mo2	O1	83.18(15)
O22	Mo2	O5	58.5(4)
O9	Mo2	O1	70.20(14)
O9	Mo2	O5	101.6(4)
O21	Mo2	O22	86.03(15)
O21	Mo2	O9	156.46(17)
O21	Mo2	O1	88.24(15)
O21	Mo2	O10	96.56(17)

Atom	Atom	Atom	Angle/°
O21	Mo2	O5	55.0(4)
O10	Mo2	O22	155.33(17)
O10	Mo2	O9	86.07(17)
O10	Mo2	O1	72.41(15)
O10	Mo2	O5	103.2(4)
O34	Mo2	O22	102.63(19)
O34	Mo2	O9	98.25(18)
O34	Mo2	O21	104.21(19)
O34	Mo2	O1	166.48(17)
O34	Mo2	O10	100.5(2)
O34	Mo2	O5	149.9(4)
O35	Mo3	O11	101.88(17)
O35	Mo3	O12	104.49(19)
O35	Mo3	O1	166.91(16)
O35	Mo3	O10	98.74(19)
O35	Mo3	O13	101.92(18)
O35	Mo3	O2	147.7(3)
O11	Mo3	O1	71.69(14)
O11	Mo3	O10	85.92(17)
O11	Mo3	O13	154.95(17)
O11	Mo3	O2	106.3(3)
O12	Mo3	O11	94.98(17)
O12	Mo3	O1	87.65(15)
O12	Mo3	O10	156.01(17)
O12	Mo3	O13	86.55(16)
O12	Mo3	O2	58.0(4)
O10	Mo3	O1	69.83(14)
O10	Mo3	O2	98.7(4)
O13	Mo3	O1	83.42(15)
O13	Mo3	O10	82.85(17)
O13	Mo3	O2	53.8(4)
O30	Mo9	O8	70.20(13)
O30	Mo9	O5	97.4(4)
O22	Mo9	O30	155.57(16)
O22	Mo9	O8	87.13(15)
O22	Mo9	O23	86.26(15)
O22	Mo9	O31	95.31(17)
O22	Mo9	O5	58.7(4)
O23	Mo9	O30	82.33(16)
O23	Mo9	O8	83.43(14)
O23	Mo9	O5	53.8(4)
O31	Mo9	O30	86.54(16)
O31	Mo9	O8	72.25(14)
O31	Mo9	O23	155.49(17)
O31	Mo9	O5	106.6(4)
O41	Mo9	O30	98.94(18)
O41	Mo9	O22	104.47(19)
O41	Mo9	O8	167.60(17)
O41	Mo9	O23	101.43(19)
O41	Mo9	O31	101.83(19)
O41	Mo9	O5	147.8(4)
O8	P1	O1	108.4(2)
O6	P1	O8	110.2(2)
O6	P1	O1	110.1(2)
O6	P1	O3	110.9(2)
O3	P1	O8	108.7(2)
O3	P1	O1	108.4(2)
O2	P1	O7	103.7(8)
O5	P1	O7	105.2(8)
O5	P1	O2	105.8(9)
O4	P1	O7	112.0(9)
O4	P1	O2	113.2(9)
O4	P1	O5	115.8(9)

Atom	Atom	Atom	Angle/°
Mo11	O26	Mo4	129.35(18)
Mo7	O18	Mo1	148.5(2)
Mo8	O20	Mo7	148.8(2)
Mo8	O32	Mo12	127.2(2)
Mo12	O27	Mo11	149.2(2)
Mo4	O24	Mo10	129.01(19)
Mo10	O25	Mo11	129.26(19)
Mo12	O30	Mo9	127.8(2)
Mo9	O22	Mo2	149.4(2)
Mo11	O29	Mo6	150.6(2)
Mo1	O19	Mo8	149.16(19)
Mo6	O28	Mo12	150.4(2)
Mo5	O14	Mo4	150.9(2)
Mo5	O16	Mo6	128.45(19)
Mo8	O8	Mo12	90.21(11)
Mo8	O8	Mo9	90.40(11)
Mo9	O8	Mo12	90.01(12)
P1	O8	Mo8	126.2(2)
P1	O8	Mo12	124.04(19)
P1	O8	Mo9	125.0(2)
Mo6	O17	Mo7	127.3(2)
Mo3	O11	Mo1	127.2(2)
Mo1	O9	Mo2	126.7(2)
Mo2	O21	Mo10	150.0(2)
Mo10	O23	Mo9	150.2(2)
Mo10	O6	Mo11	89.47(11)
Mo10	O6	Mo4	89.64(11)
Mo4	O6	Mo11	89.38(11)
P1	O6	Mo11	125.5(2)
P1	O6	Mo10	125.9(2)
P1	O6	Mo4	125.5(2)
Mo3	O12	Mo5	148.6(2)
Mo9	O31	Mo8	126.8(2)
Mo1	O1	Mo2	90.61(12)
Mo1	O1	Mo3	90.18(12)
Mo2	O1	Mo3	90.02(11)
P1	O1	Mo1	125.88(19)
P1	O1	Mo2	124.8(2)
P1	O1	Mo3	124.5(2)
Mo2	O10	Mo3	127.7(2)
Mo7	O15	Mo5	128.0(2)
Mo4	O13	Mo3	149.9(2)
Mo7	O3	Mo5	90.35(12)
Mo7	O3	Mo6	89.80(11)
Mo6	O3	Mo5	89.49(11)
P1	O3	Mo7	126.97(19)
P1	O3	Mo5	124.43(19)
P1	O3	Mo6	124.61(19)
C57	P4	C51	111.2(3)
C57	P4	C45	109.3(3)
C63	P4	C51	108.5(3)
C63	P4	C57	107.3(2)
C63	P4	C45	111.2(3)
C45	P4	C51	109.3(3)
C56	C51	P4	121.1(4)
C56	C51	C52	120.3(5)
C52	C51	P4	118.5(4)
C58	C57	P4	120.7(4)
C62	C57	P4	119.7(4)
C62	C57	C58	119.5(5)
C51	C56	C55	119.3(6)
C64	C63	P4	119.6(4)
C64	C63	C68	120.4(5)

Atom	Atom	Atom	Angle/°
C68	C63	P4	119.4(4)
C50	C45	P4	121.0(4)
C46	C45	P4	120.0(5)
C46	C45	C50	119.0(6)
C59	C58	C57	119.6(6)
C66	C65	C64	120.2(6)
C63	C64	C65	119.2(6)
C53	C52	C51	119.5(7)
C67	C68	C63	119.4(6)
C61	C62	C57	120.2(5)
C65	C66	C67	120.7(6)
C60	C61	C62	119.9(6)
C58	C59	C60	120.0(6)
C49	C50	C45	120.0(6)
C66	C67	C68	120.0(7)
C45	C46	C47	119.7(7)
C52	C53	C54	120.4(7)
C54	C55	C56	120.0(7)
C55	C54	C53	120.5(7)
C49	C48	C47	121.0(7)
C48	C49	C50	120.1(7)
C61	C60	C59	120.7(6)
C48	C47	C46	120.2(7)
C19	P2	C7	111.5(3)
C19	P2	C1	109.4(3)
C13	P2	C19	107.5(3)
C13	P2	C7	111.4(3)
C13	P2	C1	111.3(3)
C1	P2	C7	105.8(3)
C24	C19	P2	120.8(5)
C20	C19	P2	120.3(5)
C20	C19	C24	118.8(6)
C5	C6	C1	120.0(6)
C14	C13	P2	122.5(5)
C14	C13	C18	118.5(6)
C18	C13	P2	119.0(5)
C8	C7	P2	121.9(5)
C8	C7	C12	118.9(6)
C12	C7	P2	119.2(5)
C4	C5	C6	121.2(6)
C23	C24	C19	119.7(6)
C16	C15	C14	120.8(6)
C6	C1	P2	121.1(4)
C6	C1	C2	119.5(5)
C2	C1	P2	119.3(4)
C5	C4	C3	119.4(6)
C15	C14	C13	119.9(6)
C17	C16	C15	120.2(7)
C9	C8	C7	119.6(7)
C11	C12	C7	120.3(6)
C21	C20	C19	120.6(7)
C22	C23	C24	120.1(7)
C3	C2	C1	118.5(6)
C10	C9	C8	121.3(7)
C4	C3	C2	121.2(7)
C17	C18	C13	120.6(7)
C9	C10	C11	119.7(7)
C23	C22	C21	120.8(7)
C12	C11	C10	120.2(8)
C16	C17	C18	120.0(7)
C22	C21	C20	119.9(8)
C37	P3	C31	109.2(2)
C37	P3	C25	108.9(2)

Atom	Atom	Atom	Angle/°
C39	P3	C37	109.2(2)
C39	P3	C31	109.1(2)
C39	P3	C25	109.6(3)
C31	P3	C25	110.6(2)
C102	C37	P3	119.8(4)
C38	C37	P3	119.9(4)
C38	C37	C102	120.1(5)
C40	C39	P3	119.5(4)
C40	C39	C44	119.8(5)
C44	C39	P3	120.7(4)
C32	C31	P3	120.4(4)
C32	C31	C36	119.7(5)
C36	C31	P3	119.9(5)
C26	C25	P3	119.6(5)
C30	C25	P3	121.0(5)
C30	C25	C26	119.4(6)
C101	C102	C37	119.8(6)
C39	C40	C41	119.7(6)
C41	C42	C43	120.7(6)
C37	C38	C99	118.6(6)
C33	C32	C31	119.1(6)
C27	C26	C25	119.2(7)
C100	C101	C102	119.4(6)
C42	C43	C44	119.8(6)
C43	C44	C39	119.9(6)
C42	C41	C40	120.2(6)
C34	C33	C32	120.5(7)
C33	C34	C35	120.8(7)
C34	C35	C36	120.0(7)
C28	C27	C26	120.9(7)
C99	C100	C101	120.9(6)
C27	C28	C29	120.9(7)
C100	C99	C38	121.0(7)
C35	C36	C31	119.9(7)
C25	C30	C29	120.5(7)
C28	C29	C30	119.1(8)
C97	N3	C85	120.9(11)
C97	N3	C98	120.4(8)
C97	N3	C91	118.8(10)
C85	N3	C98	118.6(11)
C91	N3	C98	120.7(10)
O47	C97	N3	125.0(8)
N3	C85	C86	113.4(14)
C90	C85	N3	120.9(13)
C90	C85	C86	125.6(13)
C85	C90	C89	118.6(15)
C87	C86	C85	111.1(15)
C89	C88	C87	121.9(17)
C88	C89	C90	118.0(15)
C86	C87	C88	122.1(18)
C69	N1	C76	117.1(16)
C75	N1	C69	122(2)
C75	N1	C76	121(2)

Atom	Atom	Atom	Angle/°
C74	C69	N1	119(2)
C70	C69	N1	120(2)
C70	C69	C74	121(2)
C70	C71	C72	119.9(15)
O45	C75	N1	120(3)
C69	C74	C73	116(3)
C71	C70	C69	121.0(17)
C73	C72	C71	119(3)
C72	C73	C74	123(4)
C83	N2	C84	118(2)
C83	N2	C77	122(3)
C77	N2	C84	120(4)
C79	C78	C77	119(3)
C78	C79	C80	120.5(17)
C77	C82	C81	121(3)
C81	C80	C79	121(2)
C80	C81	C82	119(3)
O46	C83	N2	125.1(19)
C78	C77	N2	118(5)
C82	C77	N2	122(5)
C82	C77	C78	120(5)
C96	C91	N3	118.5(10)
C96	C91	C92	120.0
C92	C91	N3	121.5(10)
C95	C96	C91	120.0
C96	C95	C94	120.0
C93	C94	C95	120.0
C94	C93	C92	120.0
C93	C92	C91	120.0
Mo11	O7	Mo12	97.2(5)
Mo11	O7	Mo6	97.1(5)
Mo12	O7	Mo6	93.5(5)
P1	O7	Mo11	126.8(9)
P1	O7	Mo12	118.3(7)
P1	O7	Mo6	117.1(7)
Mo5	O2	Mo3	93.0(5)
Mo4	O2	Mo5	98.0(5)
Mo4	O2	Mo3	95.7(5)
P1	O2	Mo5	120.3(8)
P1	O2	Mo4	126.3(9)
P1	O2	Mo3	116.3(7)
Mo10	O5	Mo2	96.5(6)
Mo10	O5	Mo9	95.3(5)
Mo2	O5	Mo9	91.8(5)
P1	O5	Mo10	128.3(9)
P1	O5	Mo2	119.4(8)
P1	O5	Mo9	117.4(9)
Mo8	O4	Mo1	90.9(5)
Mo7	O4	Mo8	91.7(5)
Mo7	O4	Mo1	91.1(5)
P1	O4	Mo8	124.3(9)
P1	O4	Mo7	126.6(9)
P1	O4	Mo1	122.2(9)

Table 14: Torsion Angles in ° for **compound3**.

Atom	Atom	Atom	Atom	Angle/°
O26	Mo11	O29	Mo6	121.8(5)
O26	Mo4	O24	Mo10	65.2(2)
O26	Mo4	O13	Mo3	27.8(8)
O18	Mo7	O15	Mo5	-88.3(2)
O18	Mo1	O19	Mo8	-36.8(4)

Atom	Atom	Atom	Atom	Angle/°
O18	Mo1	O9	Mo2	5.0(6)
O20	Mo8	O32	Mo12	-88.8(3)
O20	Mo7	O18	Mo1	-36.2(4)
O20	Mo7	O15	Mo5	4.0(5)
O32	Mo8	O20	Mo7	118.2(4)
O32	Mo12	O27	Mo11	30.0(7)
O32	Mo12	O30	Mo9	68.7(3)
O27	Mo11	O26	Mo4	2.9(5)
O27	Mo11	O29	Mo6	-31.7(5)
O27	Mo12	O30	Mo9	-87.7(3)
O24	Mo10	O25	Mo11	67.2(2)
O24	Mo10	O23	Mo9	27.0(7)
O24	Mo4	O13	Mo3	121.4(5)
O25	Mo11	O26	Mo4	66.2(2)
O25	Mo11	O29	Mo6	31.0(7)
O25	Mo10	O23	Mo9	121.3(5)
O30	Mo12	O27	Mo11	123.2(4)
O30	Mo9	O22	Mo2	29.2(8)
O30	Mo9	O31	Mo8	67.7(3)
O22	Mo2	O21	Mo10	-34.8(5)
O22	Mo2	O10	Mo3	7.9(6)
O22	Mo9	O31	Mo8	-87.9(3)
O29	Mo11	O26	Mo4	-87.7(3)
O29	Mo6	O28	Mo12	-32.1(5)
O29	Mo6	O17	Mo7	3.4(5)
O35	Mo3	O11	Mo1	166.2(3)
O35	Mo3	O12	Mo5	-135.0(4)
O19	Mo8	O20	Mo7	-37.7(4)
O19	Mo8	O32	Mo12	3.9(5)
O19	Mo1	O9	Mo2	-88.5(3)
O28	Mo12	O27	Mo11	-31.3(4)
O28	Mo12	O30	Mo9	6.4(6)
O28	Mo6	O17	Mo7	-87.5(2)
O14	Mo5	O16	Mo6	-87.1(3)
O14	Mo4	O24	Mo10	-0.5(5)
O14	Mo4	O13	Mo3	-32.0(5)
O16	Mo5	O14	Mo4	123.9(4)
O16	Mo6	O28	Mo12	29.2(7)
O16	Mo6	O17	Mo7	67.4(2)
O8	Mo8	O20	Mo7	45.8(4)
O8	Mo8	O32	Mo12	-2.1(2)
O8	Mo12	O27	Mo11	51.5(4)
O8	Mo12	O30	Mo9	-1.4(2)
O8	Mo9	O22	Mo2	50.7(5)
O8	Mo9	O31	Mo8	-2.6(2)
O8	P1	O6	Mo11	-65.1(3)
O8	P1	O6	Mo10	55.0(3)
O8	P1	O6	Mo4	175.5(2)
O8	P1	O1	Mo1	55.0(3)
O8	P1	O1	Mo2	-66.2(3)
O8	P1	O1	Mo3	175.2(2)
O8	P1	O3	Mo7	-62.9(3)
O8	P1	O3	Mo5	175.4(2)
O8	P1	O3	Mo6	58.0(3)
O17	Mo7	O18	Mo1	26.3(7)
O17	Mo7	O15	Mo5	68.2(2)
O17	Mo6	O28	Mo12	123.3(5)
O11	Mo1	O19	Mo8	24.3(7)
O11	Mo1	O9	Mo2	68.6(3)
O11	Mo3	O12	Mo5	121.3(4)
O9	Mo1	O19	Mo8	119.9(4)
O9	Mo2	O21	Mo10	25.4(8)
O9	Mo2	O10	Mo3	69.6(3)

Atom	Atom	Atom	Atom	Angle/°
O21	Mo10	O25	Mo11	3.9(5)
O21	Mo10	O23	Mo9	-32.9(5)
O21	Mo2	O10	Mo3	-86.9(3)
O38	Mo6	O28	Mo12	-132.4(5)
O38	Mo6	O17	Mo7	165.5(2)
O23	Mo10	O25	Mo11	-87.0(3)
O23	Mo9	O22	Mo2	-32.9(5)
O23	Mo9	O31	Mo8	4.8(6)
O33	Mo1	O19	Mo8	-136.9(4)
O33	Mo1	O9	Mo2	166.4(3)
O6	Mo11	O26	Mo4	-3.3(2)
O6	Mo11	O29	Mo6	50.9(5)
O6	Mo10	O25	Mo11	-2.4(2)
O6	Mo10	O23	Mo9	50.0(5)
O6	Mo4	O24	Mo10	-4.4(2)
O6	Mo4	O13	Mo3	50.2(5)
O6	P1	O8	Mo8	174.9(2)
O6	P1	O8	Mo12	54.9(3)
O6	P1	O8	Mo9	-63.4(3)
O6	P1	O1	Mo1	175.7(2)
O6	P1	O1	Mo2	54.4(3)
O6	P1	O1	Mo3	-64.1(3)
O6	P1	O3	Mo7	175.8(2)
O6	P1	O3	Mo5	54.1(3)
O6	P1	O3	Mo6	-63.3(3)
O12	Mo5	O14	Mo4	-31.5(5)
O12	Mo5	O16	Mo6	6.2(6)
O12	Mo3	O11	Mo1	-87.8(3)
O31	Mo8	O20	Mo7	21.3(7)
O31	Mo8	O32	Mo12	68.4(3)
O31	Mo9	O22	Mo2	122.6(5)
O37	Mo5	O14	Mo4	-133.2(5)
O37	Mo5	O16	Mo6	167.5(3)
O1	Mo1	O19	Mo8	47.8(4)
O1	Mo1	O9	Mo2	-2.3(2)
O1	Mo2	O21	Mo10	48.5(5)
O1	Mo2	O10	Mo3	-0.8(2)
O1	Mo3	O11	Mo1	-1.9(2)
O1	Mo3	O12	Mo5	49.9(4)
O1	P1	O8	Mo8	-64.4(3)
O1	P1	O8	Mo12	175.5(2)
O1	P1	O8	Mo9	57.2(3)
O1	P1	O6	Mo11	175.4(2)
O1	P1	O6	Mo10	-64.5(3)
O1	P1	O6	Mo4	55.9(3)
O1	P1	O3	Mo7	54.7(3)
O1	P1	O3	Mo5	-67.0(3)
O1	P1	O3	Mo6	175.7(2)
O10	Mo2	O21	Mo10	120.6(5)
O10	Mo3	O11	Mo1	68.2(3)
O10	Mo3	O12	Mo5	30.2(7)
O15	Mo7	O18	Mo1	119.7(4)
O15	Mo5	O14	Mo4	32.1(7)
O15	Mo5	O16	Mo6	68.1(3)
O13	Mo4	O24	Mo10	-89.7(3)
O13	Mo3	O11	Mo1	4.7(6)
O13	Mo3	O12	Mo5	-33.6(4)
O40	Mo8	O20	Mo7	-138.5(4)
O40	Mo8	O32	Mo12	166.7(3)
O3	Mo7	O18	Mo1	48.1(4)
O3	Mo7	O15	Mo5	-2.6(2)
O3	Mo5	O14	Mo4	52.4(4)
O3	Mo5	O16	Mo6	-1.8(2)

Atom	Atom	Atom	Atom	Angle/°
O3	Mo6	O28	Mo12	51.6(5)
O3	Mo6	O17	Mo7	-2.7(2)
O3	P1	O8	Mo8	53.2(3)
O3	P1	O8	Mo12	-66.9(3)
O3	P1	O8	Mo9	174.8(2)
O3	P1	O6	Mo11	55.4(3)
O3	P1	O6	Mo10	175.5(2)
O3	P1	O6	Mo4	-64.1(3)
O3	P1	O1	Mo1	-62.8(3)
O3	P1	O1	Mo2	176.0(2)
O3	P1	O1	Mo3	57.4(3)
O42	Mo10	O25	Mo11	166.5(2)
O42	Mo10	O23	Mo9	-133.6(5)
O44	Mo12	O27	Mo11	-133.4(4)
O44	Mo12	O30	Mo9	165.8(3)
O39	Mo7	O18	Mo1	-137.5(4)
O39	Mo7	O15	Mo5	167.1(3)
O34	Mo2	O21	Mo10	-136.8(5)
O34	Mo2	O10	Mo3	167.3(3)
O36	Mo4	O24	Mo10	163.8(2)
O36	Mo4	O13	Mo3	-134.2(5)
O43	Mo11	O26	Mo4	165.4(3)
O43	Mo11	O29	Mo6	-134.0(5)
O41	Mo9	O22	Mo2	-133.7(5)
O41	Mo9	O31	Mo8	166.1(3)
P4	C51	C56	C55	-174.3(5)
P4	C51	C52	C53	174.6(5)
P4	C57	C58	C59	-179.5(5)
P4	C57	C62	C61	179.4(5)
P4	C63	C64	C65	-170.1(4)
P4	C63	C68	C67	171.3(5)
P4	C45	C50	C49	-179.5(5)
P4	C45	C46	C47	179.4(6)
C51	P4	C57	C58	67.5(6)
C51	P4	C57	C62	-113.7(5)
C51	P4	C63	C64	-155.4(4)
C51	P4	C63	C68	33.5(5)
C51	P4	C45	C50	-140.6(5)
C51	P4	C45	C46	40.6(6)
C51	C56	C55	C54	-0.1(11)
C51	C52	C53	C54	-0.1(11)
C57	P4	C51	C56	-23.1(6)
C57	P4	C51	C52	162.2(5)
C57	P4	C63	C64	84.3(5)
C57	P4	C63	C68	-86.7(5)
C57	P4	C45	C50	-18.6(6)
C57	P4	C45	C46	162.5(5)
C57	C58	C59	C60	0.4(11)
C57	C62	C61	C60	-0.2(11)
C56	C51	C52	C53	-0.2(10)
C56	C55	C54	C53	-0.2(12)
C63	P4	C51	C56	-140.9(5)
C63	P4	C51	C52	44.4(5)
C63	P4	C57	C58	-174.0(5)
C63	P4	C57	C62	4.8(6)
C63	P4	C45	C50	99.7(5)
C63	P4	C45	C46	-79.2(6)
C63	C68	C67	C66	-1.0(11)
C45	P4	C51	C56	97.7(5)
C45	P4	C51	C52	-77.0(5)
C45	P4	C57	C58	-53.3(6)
C45	P4	C57	C62	125.6(5)
C45	P4	C63	C64	-35.2(5)

Atom	Atom	Atom	Atom	Angle/°
C45	P4	C63	C68	153.8(5)
C45	C50	C49	C48	-0.4(12)
C45	C46	C47	C48	0.6(13)
C58	C57	C62	C61	-1.8(10)
C58	C59	C60	C61	-2.3(12)
C65	C66	C67	C68	0.3(11)
C64	C63	C68	C67	0.4(9)
C64	C65	C66	C67	1.0(9)
C52	C51	C56	C55	0.3(9)
C52	C53	C54	C55	0.3(13)
C68	C63	C64	C65	0.8(8)
C62	C57	C58	C59	1.7(10)
C62	C61	C60	C59	2.3(12)
C66	C65	C64	C63	-1.5(8)
C50	C45	C46	C47	0.5(11)
C46	C45	C50	C49	-0.6(10)
C49	C48	C47	C46	-1.7(15)
C47	C48	C49	C50	1.6(14)
P2	C19	C24	C23	-173.6(5)
P2	C19	C20	C21	175.6(7)
P2	C13	C14	C15	-179.8(5)
P2	C13	C18	C17	179.8(7)
P2	C7	C8	C9	-179.7(6)
P2	C7	C12	C11	-179.9(6)
P2	C1	C2	C3	174.0(6)
C19	P2	C13	C14	-130.6(6)
C19	P2	C13	C18	49.2(7)
C19	P2	C7	C8	-106.2(6)
C19	P2	C7	C12	75.4(6)
C19	P2	C1	C6	8.9(6)
C19	P2	C1	C2	-168.1(5)
C19	C24	C23	C22	-2.4(11)
C19	C20	C21	C22	-1.5(14)
C6	C5	C4	C3	-1.6(11)
C6	C1	C2	C3	-3.1(11)
C13	P2	C19	C24	-152.0(5)
C13	P2	C19	C20	33.2(6)
C13	P2	C7	C8	13.9(6)
C13	P2	C7	C12	-164.5(5)
C13	P2	C1	C6	-109.8(5)
C13	P2	C1	C2	73.2(6)
C13	C18	C17	C16	0.3(15)
C7	P2	C19	C24	-29.7(6)
C7	P2	C19	C20	155.5(6)
C7	P2	C13	C14	106.9(6)
C7	P2	C13	C18	-73.3(7)
C7	P2	C1	C6	129.1(5)
C7	P2	C1	C2	-47.9(6)
C7	C8	C9	C10	0.0(12)
C7	C12	C11	C10	-0.7(13)
C5	C6	C1	P2	-173.9(5)
C5	C6	C1	C2	3.2(9)
C5	C4	C3	C2	1.6(12)
C24	C19	C20	C21	0.6(11)
C24	C23	C22	C21	1.6(13)
C15	C16	C17	C18	-0.3(14)
C1	P2	C19	C24	87.0(5)
C1	P2	C19	C20	-87.9(6)
C1	P2	C13	C14	-10.8(7)
C1	P2	C13	C18	169.0(6)
C1	P2	C7	C8	135.0(5)
C1	P2	C7	C12	-43.4(6)
C1	C6	C5	C4	-0.9(10)

Atom	Atom	Atom	Atom	Angle/°
C1	C2	C3	C4	0.7(12)
C14	C13	C18	C17	-0.4(13)
C14	C15	C16	C17	0.3(13)
C16	C15	C14	C13	-0.4(11)
C8	C7	C12	C11	1.6(11)
C8	C9	C10	C11	0.9(13)
C12	C7	C8	C9	-1.3(10)
C20	C19	C24	C23	1.3(10)
C23	C22	C21	C20	0.3(14)
C9	C10	C11	C12	-0.5(14)
C18	C13	C14	C15	0.4(11)
P3	C37	C102	C101	-170.4(4)
P3	C37	C38	C99	171.3(5)
P3	C39	C40	C41	-178.7(5)
P3	C39	C44	C43	179.8(5)
P3	C31	C32	C33	177.6(4)
P3	C31	C36	C35	-178.3(5)
P3	C25	C26	C27	-177.6(5)
P3	C25	C30	C29	179.0(6)
C37	P3	C39	C40	-27.3(5)
C37	P3	C39	C44	153.8(5)
C37	P3	C31	C32	132.7(4)
C37	P3	C31	C36	-48.5(5)
C37	P3	C25	C26	85.2(5)
C37	P3	C25	C30	-91.4(5)
C37	C102	C101	C100	-1.4(9)
C37	C38	C99	C100	-0.4(10)
C39	P3	C37	C102	77.7(5)
C39	P3	C37	C38	-96.9(5)
C39	P3	C31	C32	13.3(5)
C39	P3	C31	C36	-167.9(5)
C39	P3	C25	C26	-155.3(4)
C39	P3	C25	C30	28.1(6)
C39	C40	C41	C42	-0.6(10)
C31	P3	C37	C102	-41.6(5)
C31	P3	C37	C38	143.7(5)
C31	P3	C39	C40	92.0(5)
C31	P3	C39	C44	-86.8(5)
C31	P3	C25	C26	-34.9(5)
C31	P3	C25	C30	148.5(5)
C31	C32	C33	C34	1.2(9)
C25	P3	C37	C102	-162.6(4)
C25	P3	C37	C38	22.8(5)
C25	P3	C39	C40	-146.7(5)
C25	P3	C39	C44	34.5(5)
C25	P3	C31	C32	-107.4(5)
C25	P3	C31	C36	71.4(5)
C25	C26	C27	C28	-0.9(10)
C25	C30	C29	C28	-2.2(12)
C102	C37	C38	C99	-3.3(9)
C102	C101	C100	C99	-2.4(10)
C40	C39	C44	C43	1.0(9)
C42	C43	C44	C39	-1.8(10)
C38	C37	C102	C101	4.2(8)
C32	C31	C36	C35	0.5(9)
C32	C33	C34	C35	-0.4(11)
C26	C25	C30	C29	2.4(10)
C26	C27	C28	C29	1.1(12)
C101	C100	C99	C38	3.3(11)
C43	C42	C41	C40	-0.3(11)
C44	C39	C40	C41	0.2(9)
C41	C42	C43	C44	1.5(11)
C33	C34	C35	C36	-0.3(12)

Atom	Atom	Atom	Atom	Angle/°
C34	C35	C36	C31	0.3(11)
C27	C28	C29	C30	0.4(12)
C36	C31	C32	C33	-1.2(8)
C30	C25	C26	C27	-0.9(9)
N3	C85	C90	C89	-175(2)
N3	C85	C86	C87	169(2)
N3	C91	C96	C95	-178.8(18)
N3	C91	C92	C93	178.7(18)
C97	N3	C85	C90	44(3)
C97	N3	C85	C86	-138.9(16)
C97	N3	C91	C96	54.5(15)
C97	N3	C91	C92	-124.3(12)
C85	N3	C97	O47	174.1(13)
C85	C90	C89	C88	-5(3)
C85	C86	C87	C88	18(4)
C98	N3	C97	O47	-1.0(13)
C98	N3	C85	C90	-140.6(18)
C98	N3	C85	C86	36(2)
C98	N3	C91	C96	-120.7(12)
C98	N3	C91	C92	60.5(18)
C90	C85	C86	C87	-14(3)
C86	C85	C90	C89	9(3)
C89	C88	C87	C86	-17(5)
C87	C88	C89	C90	9(4)
N1	C69	C74	C73	-176(3)
N1	C69	C70	C71	-179.0(19)
C69	N1	C75	O45	177(3)
C69	C74	C73	C72	-11(7)
C71	C72	C73	C74	9(7)
C75	N1	C69	C74	148(3)
C75	N1	C69	C70	-34(4)
C74	C69	C70	C71	-1(3)
C70	C69	C74	C73	7(4)
C70	C71	C72	C73	-3(5)
C72	C71	C70	C69	0(3)
C76	N1	C69	C74	-32(3)
C76	N1	C69	C70	146(2)
C76	N1	C75	O45	-3(6)
C84	N2	C83	O46	-1(4)
C84	N2	C77	C78	-25(7)
C84	N2	C77	C82	155(5)
C78	C79	C80	C81	4(5)
C79	C78	C77	N2	-180(4)
C79	C78	C77	C82	1(7)
C79	C80	C81	C82	-6(7)
C81	C82	C77	N2	178(5)
C81	C82	C77	C78	-3(8)
C83	N2	C77	C78	152(4)
C83	N2	C77	C82	-29(7)
C77	N2	C83	O46	-177(3)
C77	C78	C79	C80	-2(5)
C77	C82	C81	C80	5(8)
C91	N3	C97	O47	-176.2(12)
C91	C96	C95	C94	0.0
C96	C91	C92	C93	0.0
C96	C95	C94	C93	0.0
C95	C94	C93	C92	0.0
C94	C93	C92	C91	0.0
C92	C91	C96	C95	0.0
O7	Mo11	O26	Mo4	-30.4(4)
O7	Mo11	O29	Mo6	20.0(6)
O7	Mo12	O27	Mo11	20.0(5)
O7	Mo12	O30	Mo9	-32.5(4)

Atom	Atom	Atom	Atom	Angle/°
O7	Mo6	O28	Mo12	16.1(5)
O7	Mo6	O17	Mo7	-29.9(4)
O7	P1	O2	Mo5	-66.2(10)
O7	P1	O2	Mo4	62.9(11)
O7	P1	O2	Mo3	-177.1(8)
O7	P1	O5	Mo10	-49.1(12)
O7	P1	O5	Mo2	-176.7(8)
O7	P1	O5	Mo9	73.8(10)
O7	P1	O4	Mo8	-58.4(12)
O7	P1	O4	Mo7	65.1(12)
O7	P1	O4	Mo1	-175.2(8)
O2	Mo5	O14	Mo4	22.0(6)
O2	Mo5	O16	Mo6	-33.0(4)
O2	Mo4	O24	Mo10	-30.8(5)
O2	Mo4	O13	Mo3	18.6(6)
O2	Mo3	O11	Mo1	-29.7(5)
O2	Mo3	O12	Mo5	15.2(5)
O2	P1	O7	Mo11	-51.5(11)
O2	P1	O7	Mo12	-177.0(8)
O2	P1	O7	Mo6	72.3(10)
O2	P1	O5	Mo10	60.3(12)
O2	P1	O5	Mo2	-67.3(10)
O2	P1	O5	Mo9	-176.8(8)
O2	P1	O4	Mo8	-175.3(9)
O2	P1	O4	Mo7	-51.8(13)
O2	P1	O4	Mo1	67.9(12)
O5	Mo10	O25	Mo11	-28.0(5)
O5	Mo10	O23	Mo9	20.1(6)
O5	Mo2	O21	Mo10	19.0(6)
O5	Mo2	O10	Mo3	-31.4(5)
O5	Mo9	O22	Mo2	16.3(6)
O5	Mo9	O31	Mo8	-29.0(4)
O5	P1	O7	Mo11	59.4(11)
O5	P1	O7	Mo12	-66.1(10)
O5	P1	O7	Mo6	-176.8(8)
O5	P1	O2	Mo5	-176.6(8)
O5	P1	O2	Mo4	-47.5(12)
O5	P1	O2	Mo3	72.5(10)
O5	P1	O4	Mo8	62.3(13)
O5	P1	O4	Mo7	-174.3(9)
O5	P1	O4	Mo1	-54.5(12)
O4	Mo8	O20	Mo7	18.2(5)
O4	Mo8	O32	Mo12	-29.3(5)
O4	Mo7	O18	Mo1	19.4(5)
O4	Mo7	O15	Mo5	-27.8(4)
O4	Mo1	O19	Mo8	18.0(5)
O4	Mo1	O9	Mo2	-28.6(4)
O4	P1	O7	Mo11	-174.0(9)
O4	P1	O7	Mo12	60.5(11)
O4	P1	O7	Mo6	-50.2(11)
O4	P1	O2	Mo5	55.5(12)
O4	P1	O2	Mo4	-175.4(10)
O4	P1	O2	Mo3	-55.4(12)
O4	P1	O5	Mo10	-173.4(10)
O4	P1	O5	Mo2	59.0(12)
O4	P1	O5	Mo9	-50.5(11)

Table 15: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **compound3**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H56	418.64	9120.04	3508.12	65
H58	1957.85	8452.03	3233.2	67
H65	829.18	4409.31	4358.62	69
H64	1535.49	5668.09	4322.96	56
H52	-316.94	7855.56	4974.07	70
H68	-925.69	7055.96	4019.11	75
H62	622.23	6381.22	3037.93	61
H66	-731.3	4488.19	4257.35	78
H61	986.47	6382.31	2037.54	81
H59	2317.62	8438.54	2231.19	83
H50	2880.12	6978.86	3775.62	70
H67	-1615.25	5800.37	4090.83	84
H46	1332.04	7796.39	5198.81	82
H53	-1237.5	9091.45	5281.84	88
H55	-513.94	10362.29	3831.92	86
H54	-1329.56	10337.03	4715.79	100
H48	4074.5	7354.02	5289.65	101
H49	4192.6	6941.06	4329.34	87
H60	1784.84	7432.07	1634.4	89
H47	2666	7744.05	5736.6	105
H6	9040.1	4395.72	1349.04	58
H5	10483.4	4222.77	908.19	71
H24	8113.89	5411.61	2713.72	67
H15	6094.46	6076.77	-339.15	81
H4	11025.09	5337.3	399.45	79
H14	7363.82	5971.91	250.08	68
H16	4649.54	6064.18	69.7	85
H8	6352.9	7397.19	1724.17	75
H12	8954.25	6542.57	2172.24	85
H20	6909.46	4212.11	1449.01	92
H23	8128.33	4178.33	3306.75	85
H2	8633.33	6848.28	730.13	82
H9	6437.52	8652.88	2229.06	96
H3	10093.46	6636.36	293.26	94
H18	5696.78	5858.77	1675.3	103
H10	7737.76	8853.04	2712.22	99
H22	7472.02	3019.98	2990.23	97
H11	9006.95	7797.61	2679.57	98
H17	4443.18	5964.1	1072.04	107
H21	6859.6	3031.35	2069.26	107
H102	5657.23	1061.51	773.76	57
H40	6370.06	710.72	1821.99	63
H42	8003.02	998.67	3174.41	77
H38	7123.53	-1300.29	641.5	65
H32	7924.1	2120.35	1087.95	56
H26	8444.98	78.87	-314.02	66
H101	4303.66	436.29	817.63	71
H43	9290.58	735.15	2559.24	73
H44	9121.87	512.7	1560.42	63
H41	6552.85	979.83	2814.43	79
H33	7880.13	3405.09	549.65	73
H34	7401.09	3481.81	-404.88	87
H35	6977.2	2287.63	-849.64	95
H27	9633.52	-914.73	-680.38	86
H100	4372.62	-1046.45	792.47	86
H28	10441.21	-1881.2	-69.71	99
H99	5744.07	-1897.67	663.08	86
H36	7040.21	988.53	-336.76	72
H30	8841.96	-975.1	1301.33	76
H29	10071.02	-1921.29	926.28	103
H97	4611.17	8315.4	2115.01	90
H98A	3632.32	6397.96	2792.79	158
H98B	4603.02	5937.92	2580.64	158

Atom	x	y	z	U_{eq}
H98C	3888.56	6338.12	2115.07	158
H90	4510.55	8601.52	3138.62	92
H86	5575.28	6030.93	3078.54	130
H88	6518.7	7638.53	4216.85	129
H89	5565.5	8831.74	3860.67	115
H87	6785.05	6394.14	3666.94	146
H71	2811.1	823.16	5045.14	97
H75	5348.48	505.28	3941.7	99
H74	5549.49	-726.37	5660.04	93
H70	4172.62	1005.25	4569.29	107
H72	2797.63	-155.12	5829.29	120
H76A	6467.61	338.92	5499.74	183
H76B	7056.06	561.13	4940.12	183
H76C	6927.71	-404.87	5086.69	183
H73	4115.77	-1048.06	6027.27	132
H84A	4230.06	5906.21	6045.84	119
H84B	4816.15	4994.49	6123.86	119
H84C	3736.46	5088.33	6188.83	119
H78	5706.53	5753.35	5532.15	81
H79	7034.51	5651.41	4935.14	109
H82	4568.39	4333.13	4366.02	77
H80	7144.24	4836.97	4082.95	119
H81	5884.94	4295.59	3750.71	108
H83	3311.36	5043.85	4737.01	87
H96	4046.26	8553.7	3191.97	122
H95	4745.14	8984.42	4025.68	149
H94	6051.47	8149.92	4382.12	161
H93	6658.94	6884.7	3904.85	159
H92	5960.07	6453.97	3071.14	127

Table 16: Atomic Occupancies for all atoms that are not fully occupied in **compound3**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
O8	0.8	H76B	0.5	C93	0.51(3)
O6	0.8	H76C	0.5	H93	0.51(3)
O1	0.8	C73	0.5	C92	0.51(3)
O3	0.8	H73	0.5	H92	0.51(3)
C85	0.49(3)	O46	0.5	O7	0.2
C90	0.49(3)	N2	0.5	O2	0.2
H90	0.49(3)	C84	0.5	O5	0.2
C86	0.49(3)	H84A	0.5	O4	0.2
H86	0.49(3)	H84B	0.5		
C88	0.49(3)	H84C	0.5		
H88	0.49(3)	C78	0.5		
C89	0.49(3)	H78	0.5		
H89	0.49(3)	C79	0.5		
C87	0.49(3)	H79	0.5		
H87	0.49(3)	C82	0.5		
O45	0.5	H82	0.5		
N1	0.5	C80	0.5		
C69	0.5	H80	0.5		
C71	0.5	C81	0.5		
H71	0.5	H81	0.5		
C75	0.5	C83	0.5		
H75	0.5	H83	0.5		
C74	0.5	C77	0.5		
H74	0.5	C91	0.51(3)		
C70	0.5	C96	0.51(3)		
H70	0.5	H96	0.51(3)		
C72	0.5	C95	0.51(3)		
H72	0.5	H95	0.51(3)		
C76	0.5	C94	0.51(3)		
H76A	0.5	H94	0.51(3)		

Citations

O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.

SADABS, Bruker axs, Madison, WI (?).

Sheldrick, G.M., Crystal structure refinement with ShelXL, *Acta Cryst.*, (2015), **C71**, 3-8.

Sheldrick, G.M., ShelXT-Integrated space-group and crystal-structure determination, *Acta Cryst.*, (2015), **A71**, 3-8.

Packing diagrams for compounds **1**, **2** and **3** are shown in **Figures S5, S6 and S7**

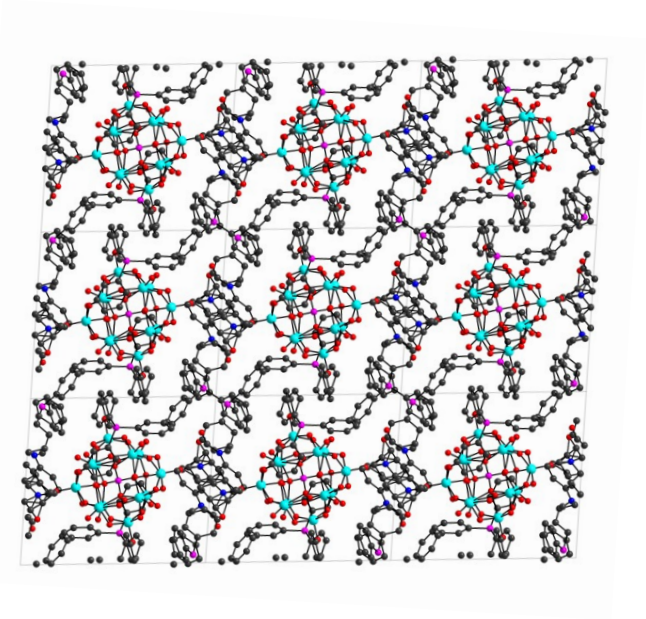


Fig. 1. **S** ons in the crystal structure of compound

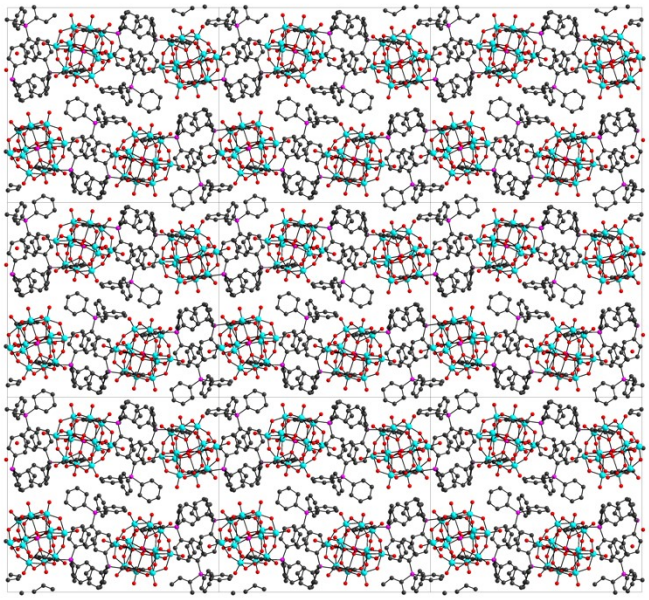


Fig. S6. The packing of tetraphenylphosphonium cations and Keggin anions in the crystal structure of compound **2.**

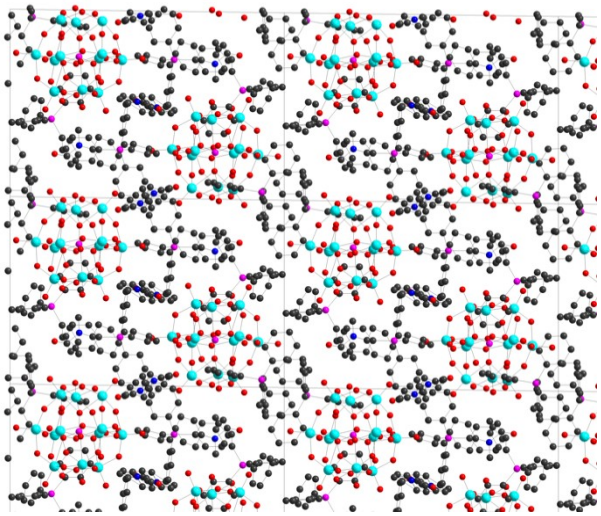


Fig. S7. The packing of tetraphenylphosphonium cations and Keggin anions in the crystal structure of compound **3**.

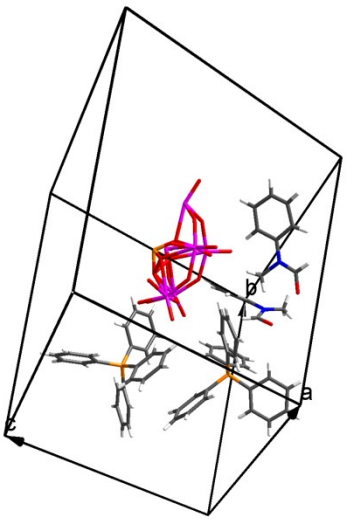


Fig. S8. Left: The asymmetric unit in the crystal structure of compound **1**.

S5. Thermogravimetric Analysis (TGA)

The TGA data was recorded on a Mettler Toledo TGA 1 instrument for the temperature range of 25˚-800˚C at the rate of 5˚C min^{-1} under an inert flow of dry N_2 gas (flow rate 20 $cm^3\,min^{-1}$). Prior to recording the data for the solid sample, a blank was run under the same parameters using an empty ceramic crucible.

S5.1. The thermogravimetric analysis for compounds **1** shows the loss of two NMF molecules in the temperature range of 130-150˚C.

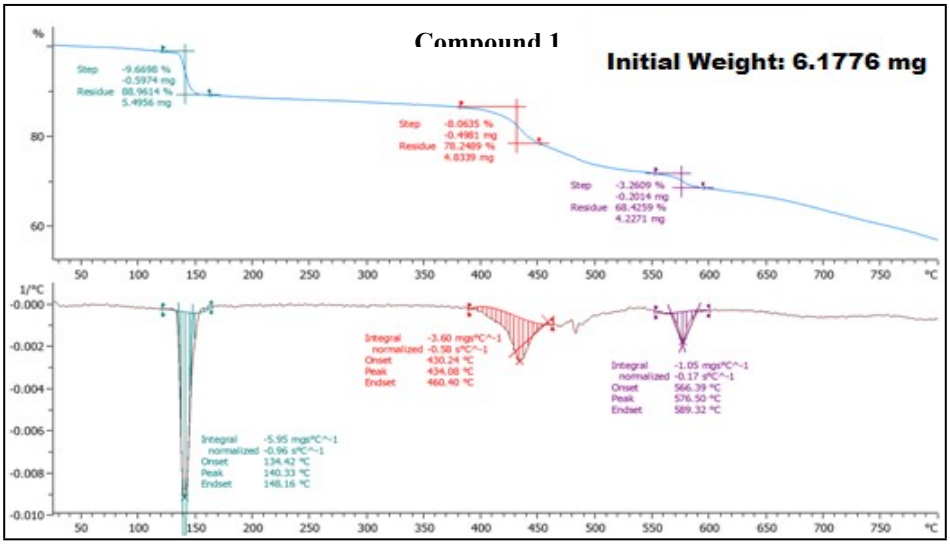


Fig. S9. Thermal analysis plot for compound **1**.

S5.2. The thermogravimetric analysis for compound **2** showed minimal weight loss before 400˚C. The framework disintegration was observed beyond 450˚C.

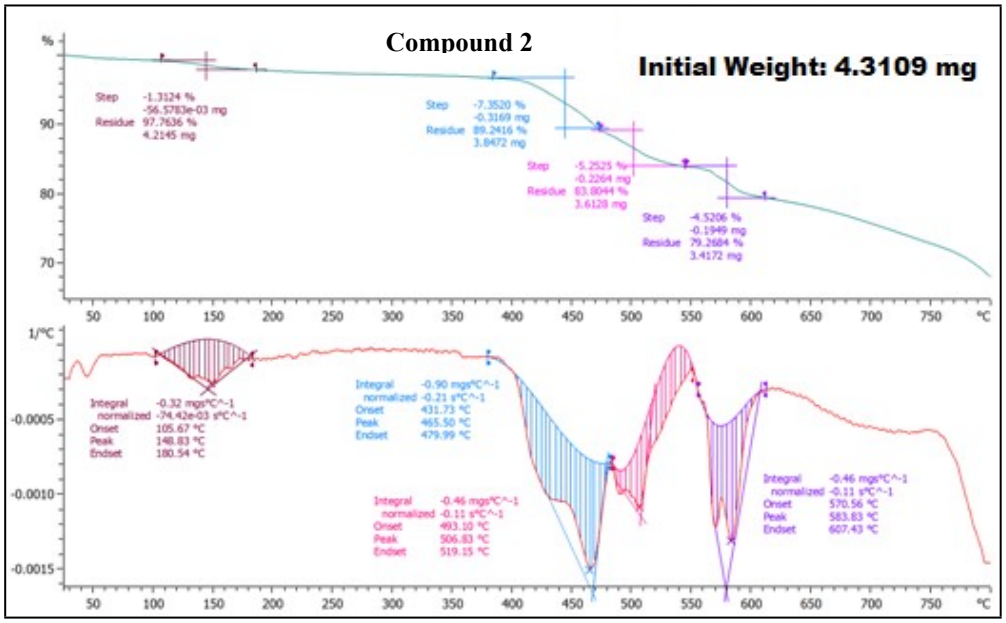


Fig. S10. Thermal analysis plot for compound **2**.

S6. The thermogravimetric analysis for compounds **3** shows the loss of one NMF molecule in the temperature range of 130-150˚C.

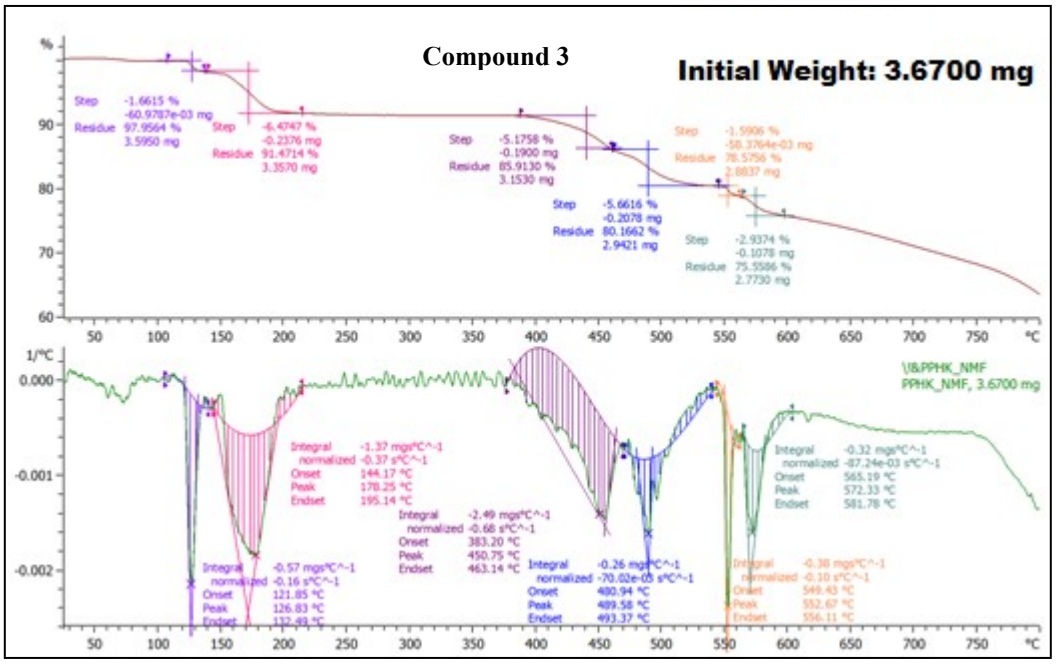


Fig. S11. Thermal analysis plot for compound **3**.

S6. Electron Paramagnetic Resonance Spectroscopy (EPR)

The room temperature EPR spectra of reduced compound **1** is shown in Fig. S13.

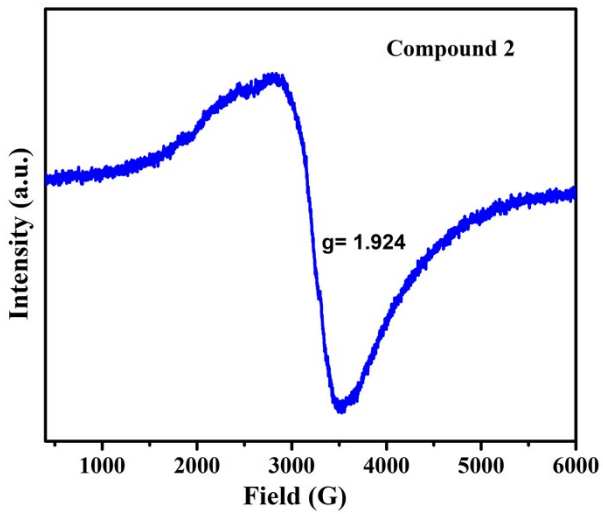
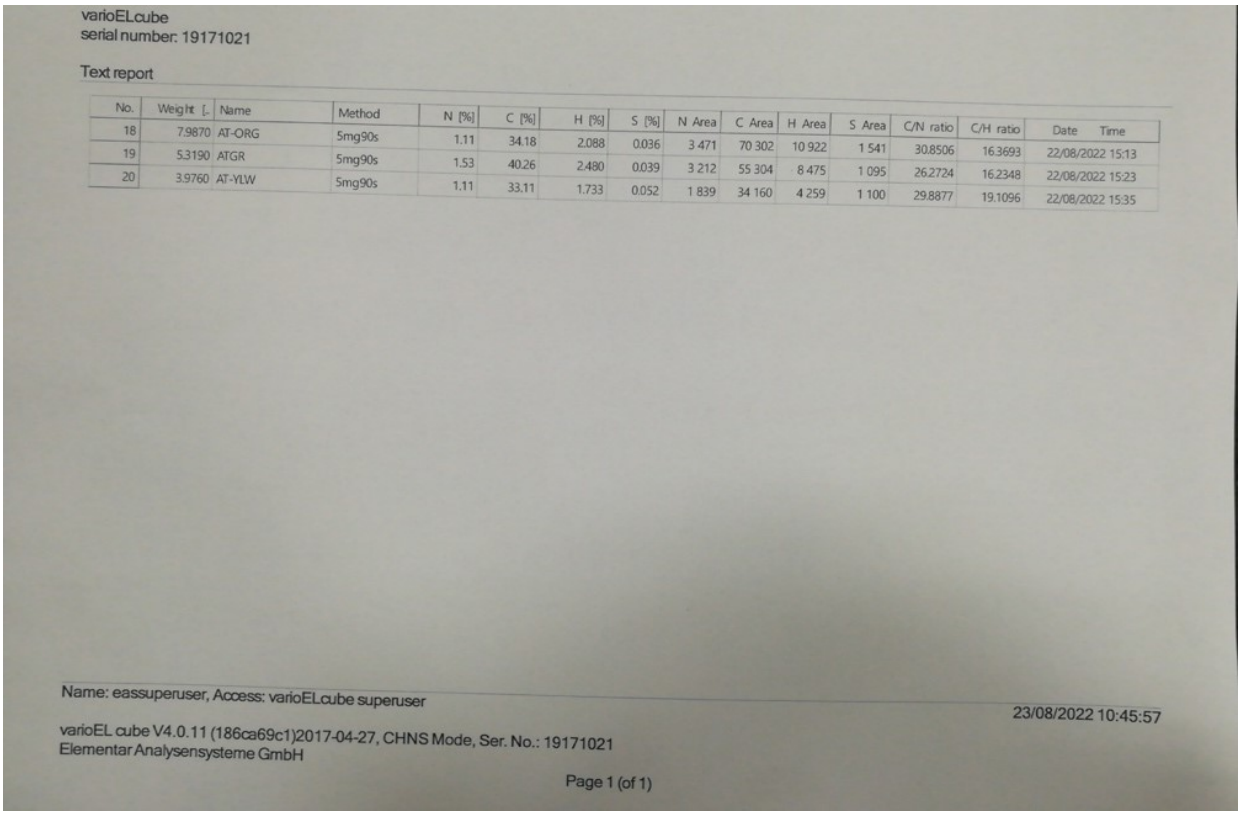


Fig. S12. The room temperature EPR spectra of green crystalline solid of compound **1**.

S7. Elemental analysis

The CHN data of compounds **1**, **2** and **3** are given in **Fig. S14** and data were collected on Elementar, Vario EL Cube instrument. The compound **1** shows presence of four solvent methyl formanilide molecules as observed from the CHN data. The crystal structure of compound **2** is solved and refined by applying SQUEEZ command therefore the solvent molecules are not given in the crystal data but solvent molecules are mentioned in the formulas of compound **2** based on CHN data.



varioELcube
serial number: 19171021

Text report

No.	Weight [..	Name	Method	N [%]	C [%]	H [%]	S [%]	N Area	C Area	H Area	S Area	C/N ratio	C/H ratio	Date	Time
18	7.9870	AT-ORG	5mg90s	1.11	34.18	2.088	0.036	3 471	70 302	10 922	1 541	30.8506	16.3693	22/08/2022	15:13
19	5.3190	ATGR	5mg90s	1.53	40.26	2.480	0.039	3 212	55 304	8 475	1 095	26.2724	16.2348	22/08/2022	15:23
20	3.9760	AT-YLW	5mg90s	1.11	33.11	1.733	0.052	1 839	34 160	4 259	1 100	29.8877	19.1096	22/08/2022	15:35

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23/08/2022 10:45:57

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Page 1 (of 1)

The observed and calculated CHN data for compounds **1**, **2** and **3** are given below.

Compound **1** $[PPh_4]_4[PMo^{V}Mo^{VI}_{11}O_{40}] \cdot 3CH_3(C_6H_5)NCHO$

Anal. Calcd. for $C_{120}H_{107}N_3O_{43}P_5Mo_{12}$: C, 40.26 (40.20); H, 2.48 (3.01); N, 1.53 (1.17).

Compound **2** $[PPh_4]_3[PMo^{VI}_{12}O_{40}] \cdot 3CH_3(C_6H_5)NCHO$

Anal. Calcd. for $C_{96}H_{87}N_3O_{43}P_4Mo_{12}$: C, 33.11 (35.52); H, 1.73(2.70); N, 1.11 (1.29).

Compound **3** $[PPh_4]_3[PMo^{VI}_{12}O_{40}] \cdot 2CH_3(C_6H_5)NCHO$

Anal. Calcd. for $C_{88}H_{78}N_2O_{42}P_4Mo_{12}$: C, 34.18 (33.98); H, 2.09(2.53); N, 1.11(0.90).

S8. Synthetic procedures

8.1. Synthesis of polycrystalline compound.

Aqueous solution of $H_3[PMo_{12}O_{40}]$ (0.70g, 0.42mmol in 75ml) was prepared. To it 25mL H_2O-MeOH (4:1 v/v) solution of tetraphenylphosphonium bromide; PPh_4Br (1.5g, 3.5mmol) was added. The obtained yellow colored suspension was refluxed for two hours

at 100˚C. Resultant yellow precipitate was washed with water and vacuum dried. Yield: 89.6%. IR (cm^{-1}): 1435 (s, ν(C=C)), 1104 (s, ν_s(P-C)), 1060 (m, $\nu_{as}(PO_4)$), 952 (m, ν(Mo=O_t)), 879 (s), 794 (s), 714 (m), 680 (s, ν(C-H)), 522 (s), 408 (s).

8.2. Synthesis of Compound 1

A 4 mL suspension of polycrystalline compound (81.1 μmol, 0.25 g) in N-methylformanilide (NMF) was sonicated for thirty minutes. The obtained suspension was then irradiated with sunlight. After fifteen minutes green needle shape crystals were obtained. The crystals were separated, washed and dried. IR (cm^{-1}): 1670 (s, ν(C=O)), 1593 (s), 1497 (s), 1437 (s, ν(C=C)), 1347 (m), 1323 (m), 1266 (m), 1189 (m), 1165 (s), 1108 (s, ν_s(P-C)), 1060 (m, $\nu_{as}(PO_4)$), 1027 (m), 997 (m), 955 (m, ν(Mo=O_t)), 877 (s), 802 (s), 743 (m), 719 (m), 689 (s, ν(C-H)), 527 (s), 459 (m).

8.3. Synthesis of Compound 2

After the separation of compound **1** from the polycrystalline suspension in NMF, the solvent was filtered to remove the undissolved compound polycrystalline compound. The clear yellow filtrate was then allowed to stand at low temperature (~ 10˚C). Yellow plate shape crystals were obtained after 7 days. IR (cm^{-1}): 1482 (m), 1437 (s, ν(C=C)), 1323 (m), 1189 (m), 1162 (m), 1108 (s, ν_s(P-C)), 1060 (m, $\nu_{as}(PO_4)$), 997 (m), 952 (m, ν(Mo=O_t)), 877 (s), 797 (s), 746 (m), 719 (m), 686 (s, ν(C-H)), 524 (s), 461 (m).

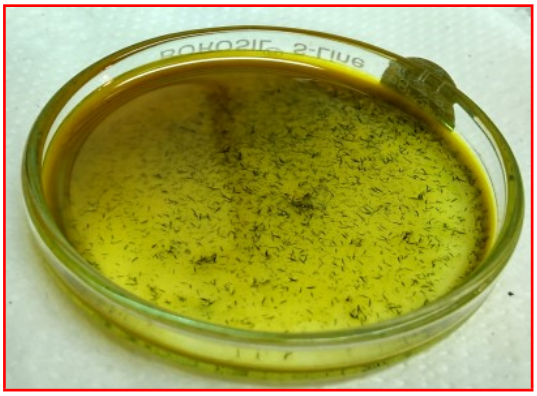
8.4. Synthesis of Compound 3

After the separation of compound **1** from suspension in NMF, the solvent was filtered to remove the undissolved polycrystalline compound. The clear yellow filtrate was then allowed to stand undisturbed at room temperature. Orange cube shape crystals were obtained after 4 days.

IR (cm^{-1}): 1670 (s, ν(C=O)), 1589 (s), 1497 (s), 1434 (s, ν(C=C)), 1350 (m), 1320 (m), 1266 (m), 1191 (m), 1162 (s), 1108 (s, ν_s(P-C)), 1060 (m, $\nu_{as}(PO_4)$), 1027 (m), 994 (m), 955 (m, ν(Mo=O_t)), 880 (s), 802 (s), 746 (m), 719 (m), 686 (s, ν(C-H)), 524 (s), 461 (m).

S8. The real time images of initiation of crystallization and green crystal of compound 1

Initiation of crystallization



Green crystals formed along with the yellow amorphous compound which remains undissolved

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