mo_B1959_0m

Table S1 Crystal data and structure refinement for mo_B1959_0m.

Identification code	mo_B1959_0m
Empirical formula	$C_{29}H_{15}Co_4O_{14}P$
Formula weight	854.10
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.5987(10)
b/Å	8.9773(9)
c/Å	27.953(2)
α/°	90
β/°	96.829(3)
γ/°	90
Volume/Å^3	3139.2(5)
Z	4
ρ_{calc}g/cm^3	1.807
μ/mm^{-1}	2.198
F(000)	1696.0
Crystal size/mm^3	0.377 × 0.194 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.768 to 66.294
Index ranges	$-19 \leq h \leq 19$, $-13 \leq k \leq 13$, $-42 \leq l \leq 39$
Reflections collected	80868
Independent reflections	11958 [R_{int} = 0.0294, R_{sigma} = 0.0190]
Data/restraints/parameters	11958/0/461
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0236, wR_2 = 0.0546
Final R indexes [all data]	R_1 = 0.0296, wR_2 = 0.0579
Largest diff. peak/hole / e Å^{-3}	0.58/-0.41

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for mo_B1959_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Co1	6287.1(2)	2351.0(2)	3898.6(2)	16.53(3)
Co2	5487.3(2)	4855.4(2)	3813.6(2)	15.70(3)
Co2A	4722(4)	3732(5)	4146.7(16)	22.6(10)
Co3	5319.2(2)	3145.8(2)	3125.8(2)	15.51(3)
Co3A	5550(4)	4329(5)	3398.1(16)	22.6(10)
Co4	4295.7(2)	2610.9(2)	3825.2(2)	17.46(4)

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for mo_B1959_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Co4A	4546(4)	1942(5)	3471.0(17)	23.2(10)
P1	7971.6(2)	2586.5(3)	3846.9(2)	17.26(5)
O1	8340.1(7)	4234.6(10)	4015.5(3)	22.58(16)
O2	8347.0(7)	2513.0(10)	3319.4(3)	22.21(16)
O3	8861.5(6)	1528.1(10)	4127.6(3)	22.62(17)
O4	6033.7(9)	39.7(11)	3153.3(4)	31.6(2)
O5	6093.8(8)	-152.6(14)	4547.0(5)	47.3(3)
O6	6633.2(7)	4189.4(12)	4766.9(3)	27.83(19)
O7	6855.1(8)	3886.8(11)	2452.1(3)	28.31(19)
O8	7063.3(8)	7171.1(12)	3680.3(4)	33.7(2)
O9	4165.2(8)	5971.9(10)	2958.1(3)	25.89(18)
O10	4053.2(8)	6717.1(12)	4304.2(4)	32.9(2)
O11	2290.9(8)	3928.0(13)	3360.9(4)	35.1(2)
O12	4097.7(8)	2875.4(13)	4867.8(4)	32.8(2)
O13	3727.0(10)	-566.2(13)	3662.3(4)	40.9(3)
O14	3549.5(8)	2132.6(11)	2434.3(4)	29.7(2)
C1	9351.4(9)	4861.0(13)	3985.6(5)	22.0(2)
C2	9490.2(11)	5752.3(16)	3595.9(5)	30.2(3)
C3	10469.4(13)	6465.9(18)	3590.2(7)	40.2(4)
C4	11278.4(12)	6276.7(18)	3965.5(7)	40.6(4)
C5	11127.3(11)	5363.5(18)	4347.5(6)	36.4(3)
C6	10150.5(10)	4645.1(15)	4362.4(5)	26.9(2)
C7	9070.1(9)	1516.0(14)	3147.4(4)	20.7(2)
C8	10157.0(10)	1677.5(16)	3280.4(6)	29.2(3)
C9	10854.0(11)	729.4(17)	3076.5(6)	32.3(3)
C10	10472.5(12)	-341.3(18)	2750.0(5)	34.4(3)
C11	9382.8(14)	-486(2)	2625.4(7)	50.1(5)
C12	8672.4(12)	452(2)	2823.6(6)	40.0(4)
C13	8685.2(8)	573.0(13)	4506.2(4)	18.73(19)
C14	8655.4(10)	-937.9(14)	4416.2(5)	23.8(2)
C15	8499.5(11)	-1903.6(15)	4789.6(5)	28.5(3)
C16	8393.8(10)	-1357.7(16)	5243.6(5)	27.4(2)
C17	8443.0(11)	163.3(16)	5328.4(5)	29.0(3)
C18	8587.7(11)	1143.6(15)	4957.7(5)	26.0(2)
C19	5952.7(9)	1211.0(13)	3320.0(4)	21.9(2)
C20	6226.8(9)	817.7(16)	4299.8(5)	27.8(3)
C21	6310.9(9)	3892.7(14)	4373.4(4)	20.7(2)
C22	6467.9(10)	6263.8(14)	3733.9(4)	23.5(2)
C23	6267.7(9)	3609.5(13)	2712.7(4)	21.6(2)
C24	4712.7(9)	5121.4(13)	3178.4(4)	19.2(2)
C25	4615.3(10)	5979.6(15)	4125.6(4)	24.2(2)
C26	3055.9(10)	3438.0(14)	3551.3(5)	24.1(2)

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for mo_B1959_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C27	4168.6(10)	2762.8(15)	4469.3(5)	25.0(2)
C28	3956.8(10)	643.2(16)	3721.2(5)	27.3(2)
C29	4250.8(10)	2500.1(13)	2699.5(4)	22.3(2)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for mo_B1959_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	14.81(6)	16.72(7)	17.84(7)	2.94(5)	0.98(5)	2.55(5)
Co2	16.55(7)	15.47(7)	14.72(7)	-0.31(5)	0.39(5)	2.05(5)
Co2A	21(2)	26(2)	21(2)	-0.3(16)	2.3(15)	4.0(16)
Co3	17.49(7)	14.61(7)	14.21(7)	0.28(5)	0.98(5)	1.02(5)
Co3A	28(2)	21(2)	19.1(19)	0.5(15)	1.3(16)	-3.5(16)
Co4	14.78(7)	19.11(7)	18.44(7)	2.99(5)	1.77(5)	0.91(5)
Co4A	25(2)	21(2)	22(2)	-3.3(16)	-0.9(16)	-1.6(16)
P1	15.73(11)	17.98(13)	18.02(12)	1.89(10)	1.83(9)	2.59(9)
O1	18.3(4)	19.9(4)	30.2(4)	-2.4(3)	5.1(3)	0.0(3)
O2	21.8(4)	26.4(4)	18.8(4)	2.4(3)	4.0(3)	7.0(3)
O3	17.4(3)	27.1(4)	23.4(4)	8.2(3)	2.6(3)	5.0(3)
O4	42.2(5)	20.4(4)	31.4(5)	-2.2(4)	1.1(4)	7.3(4)
O5	24.6(5)	50.7(7)	65.9(8)	39.1(6)	2.9(5)	2.1(5)
O6	26.9(4)	38.0(5)	17.6(4)	-1.7(4)	-1.3(3)	7.3(4)
O7	29.9(4)	28.6(5)	27.4(4)	0.9(4)	7.4(4)	-1.6(4)
O8	31.3(5)	26.6(5)	40.5(6)	3.1(4)	-7.4(4)	-6.3(4)
O9	31.4(4)	22.4(4)	22.8(4)	2.3(3)	-1.1(3)	5.7(3)
O10	38.0(5)	35.8(5)	25.6(5)	-1.6(4)	7.4(4)	15.1(4)
O11	23.0(4)	40.4(6)	40.1(6)	-1.0(5)	-3.0(4)	5.8(4)
O12	33.9(5)	38.2(6)	26.7(5)	1.6(4)	4.9(4)	-3.5(4)
O13	49.0(6)	27.5(5)	44.6(6)	3.3(5)	-1.0(5)	-4.3(5)
O14	31.4(5)	28.0(5)	28.0(5)	-2.6(4)	-3.9(4)	-5.0(4)
C1	18.8(5)	18.8(5)	28.6(6)	-4.1(4)	4.3(4)	0.2(4)
C2	29.5(6)	26.2(6)	35.7(7)	3.9(5)	6.7(5)	-0.3(5)
C3	37.9(8)	28.3(7)	57.8(10)	3.3(7)	20.3(7)	-4.7(6)
C4	25.2(6)	27.8(7)	70.8(11)	-15.5(7)	14.0(7)	-6.5(5)
C5	22.8(6)	33.7(7)	51.2(9)	-17.9(7)	-1.5(6)	0.9(5)
C6	24.2(5)	26.9(6)	28.9(6)	-6.8(5)	0.4(5)	2.8(5)
C7	20.1(5)	23.9(5)	18.7(5)	2.4(4)	4.5(4)	4.4(4)
C8	20.6(5)	26.0(6)	42.1(7)	-4.0(5)	7.5(5)	-1.7(4)
C9	21.1(5)	31.1(7)	46.6(8)	2.0(6)	11.9(5)	1.8(5)
C10	34.7(7)	41.1(8)	28.4(6)	-1.3(6)	7.8(5)	15.7(6)
C11	41.0(8)	62.9(12)	42.9(9)	-31.0(8)	-9.3(7)	18.4(8)

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for mo_B1959_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C12	27.0(6)	53.6(10)	36.5(7)	-20.2(7)	-7.9(5)	11.1(6)
C13	14.4(4)	21.2(5)	19.9(5)	3.1(4)	-0.8(4)	2.6(4)
C14	22.6(5)	22.8(5)	25.4(5)	-2.8(4)	0.5(4)	2.2(4)
C15	27.4(6)	19.1(5)	38.4(7)	3.1(5)	1.1(5)	1.7(4)
C16	22.5(5)	29.8(6)	29.5(6)	10.8(5)	1.3(4)	1.2(5)
C17	34.5(6)	32.2(7)	20.5(5)	0.9(5)	3.9(5)	-1.8(5)
C18	32.3(6)	21.3(5)	24.9(6)	-1.8(4)	5.0(5)	-0.9(5)
C19	22.6(5)	19.1(5)	24.1(5)	1.1(4)	3.0(4)	2.1(4)
C20	17.0(5)	30.7(6)	35.3(7)	11.7(5)	0.8(4)	3.9(4)
C21	17.0(4)	25.8(6)	19.3(5)	2.6(4)	2.2(4)	3.6(4)
C22	23.7(5)	22.3(5)	23.1(5)	0.6(4)	-2.7(4)	3.2(4)
C23	22.9(5)	18.0(5)	23.3(5)	0.8(4)	-0.1(4)	0.7(4)
C24	21.4(5)	18.3(5)	17.7(5)	-0.1(4)	2.2(4)	-0.6(4)
C25	26.7(5)	26.0(6)	18.8(5)	0.0(4)	-1.4(4)	5.0(4)
C26	21.9(5)	24.6(6)	25.8(5)	-0.8(4)	2.8(4)	-0.2(4)
C27	19.2(5)	28.4(6)	27.6(6)	5.7(5)	3.4(4)	0.3(4)
C28	24.9(5)	28.3(6)	28.4(6)	6.6(5)	2.0(5)	0.9(5)
C29	26.3(5)	18.8(5)	21.6(5)	-1.1(4)	1.7(4)	1.1(4)

Table S4 Bond Lengths for mo_B1959_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	Co2	2.4637(3)	O2	C7	1.4023(14)
Co1	Co2A	2.496(4)	O3	C13	1.4002(14)
Co1	Co3	2.4568(3)	O4	C19	1.1595(15)
Co1	Co3A	2.380(5)	O5	C20	1.1365(16)
Co1	Co4	2.5037(3)	O6	C21	1.1575(14)
Co1	Co4A	2.399(5)	O7	C23	1.1264(15)
Co1	P1	2.1546(4)	O8	C22	1.1293(16)
Co1	C19	1.9181(12)	O9	C24	1.1563(14)
Co1	C20	1.7828(13)	O10	C25	1.1284(15)
Co1	C21	1.9153(12)	O11	C26	1.1330(15)
Co2	Co3	2.4494(3)	O12	C27	1.1325(16)
Co2	Co4	2.5152(3)	O13	C28	1.1306(18)
Co2	C21	1.9712(11)	O14	C29	1.1328(15)
Co2	C22	1.8000(13)	C1	C2	1.3796(19)
Co2	C24	1.9365(11)	C1	C6	1.3814(18)
Co2	C25	1.7928(13)	C2	C3	1.392(2)
Co2A	Co3A	2.505(6)	C3	C4	1.383(3)
Co2A	Co4A	2.470(6)	C4	C5	1.377(3)
Co3	Co4	2.5129(3)	C5	C6	1.3944(19)
Co3	C19	1.9610(12)	C7	C8	1.3832(17)

Table S4 Bond Lengths for mo_B1959_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co3	C23	1.8063(12)	C7	C12	1.3693(19)
Co3	C24	1.9436(12)	C8	C9	1.3926(19)
Co3	C29	1.7852(12)	C9	C10	1.372(2)
Co3A	Co4A	2.510(7)	C10	C11	1.382(2)
Co4	C26	1.8147(13)	C11	C12	1.391(2)
Co4	C27	1.8315(13)	C13	C14	1.3793(17)
Co4	C28	1.8325(14)	C13	C18	1.3809(17)
P1	O1	1.6046(9)	C14	C15	1.3886(19)
P1	O2	1.6025(9)	C15	C16	1.382(2)
P1	O3	1.6020(9)	C16	C17	1.386(2)
O1	C1	1.4042(14)	C17	C18	1.3878(18)

Table S5 Bond Angles for mo_B1959_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Co2	Co1	Co4	60.835(6)	C29	Co3	C23	98.72(6)
Co3	Co1	Co2	59.708(6)	C29	Co3	C24	94.29(5)
Co3	Co1	Co4	60.865(7)	Co1	Co3A	Co2A	61.40(15)
Co3A	Co1	Co2A	61.76(16)	Co1	Co3A	Co4A	58.68(15)
Co3A	Co1	Co4A	63.36(16)	Co2A	Co3A	Co4A	59.02(18)
Co4A	Co1	Co2A	60.57(15)	Co1	Co4	Co2	58.796(7)
P1	Co1	Co2	107.385(11)	Co1	Co4	Co3	58.646(7)
P1	Co1	Co2A	141.88(11)	Co3	Co4	Co2	58.305(7)
P1	Co1	Co3	107.602(11)	C26	Co4	Co1	151.23(4)
P1	Co1	Co3A	101.88(11)	C26	Co4	Co2	98.74(4)
P1	Co1	Co4	166.108(11)	C26	Co4	Co3	95.11(4)
P1	Co1	Co4A	146.25(11)	C26	Co4	C27	102.29(6)
C19	Co1	Co2	111.05(4)	C26	Co4	C28	98.90(6)
C19	Co1	Co3	51.48(4)	C27	Co4	Co1	97.49(4)
C19	Co1	Co4	82.13(4)	C27	Co4	Co2	94.31(4)
C19	Co1	P1	96.61(4)	C27	Co4	Co3	149.71(4)
C20	Co1	Co2	135.87(5)	C27	Co4	C28	100.48(6)
C20	Co1	Co2A	96.58(12)	C28	Co4	Co1	97.79(4)
C20	Co1	Co3	136.34(4)	C28	Co4	Co2	153.95(4)
C20	Co1	Co3A	154.56(12)	C28	Co4	Co3	101.08(4)
C20	Co1	Co4	90.36(4)	Co1	Co4A	Co2A	61.67(15)
C20	Co1	Co4A	95.18(12)	Co1	Co4A	Co3A	57.96(15)
C20	Co1	P1	103.53(4)	Co2A	Co4A	Co3A	60.38(18)
C20	Co1	C19	95.57(6)	O1	P1	Co1	108.89(3)
C20	Co1	C21	96.92(6)	O2	P1	Co1	117.29(4)
C21	Co1	Co2	51.68(3)	O2	P1	O1	101.62(5)
C21	Co1	Co3	111.38(3)	O3	P1	Co1	123.13(4)
C21	Co1	Co4	85.55(3)	O3	P1	O1	104.00(5)

Table S5 Bond Angles for mo_B1959_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C21	Co1	P1	92.36(3)	O3	P1	O2	99.22(5)
C21	Co1	C19	162.49(5)	C1	O1	P1	125.78(7)
Co1	Co2	Co4	60.369(9)	C7	O2	P1	128.07(8)
Co3	Co2	Co1	60.008(8)	C13	O3	P1	124.66(7)
Co3	Co2	Co4	60.801(7)	C2	C1	O1	118.70(11)
C21	Co2	Co1	49.66(4)	C2	C1	C6	122.29(12)
C21	Co2	Co3	109.67(4)	C6	C1	O1	118.86(11)
C21	Co2	Co4	84.10(4)	C1	C2	C3	118.14(14)
C22	Co2	Co1	111.97(4)	C4	C3	C2	120.59(15)
C22	Co2	Co3	109.85(4)	C5	C4	C3	120.25(13)
C22	Co2	Co4	169.67(4)	C4	C5	C6	120.16(14)
C22	Co2	C21	95.85(5)	C1	C6	C5	118.56(14)
C22	Co2	C24	94.49(5)	C8	C7	O2	120.25(11)
C24	Co2	Co1	110.90(4)	C12	C7	O2	118.06(11)
C24	Co2	Co3	50.98(3)	C12	C7	C8	121.56(12)
C24	Co2	Co4	82.77(3)	C7	C8	C9	118.58(13)
C24	Co2	C21	160.42(5)	C10	C9	C8	120.80(13)
C25	Co2	Co1	137.23(4)	C9	C10	C11	119.51(13)
C25	Co2	Co3	137.20(4)	C10	C11	C12	120.62(15)
C25	Co2	Co4	92.49(4)	C7	C12	C11	118.92(14)
C25	Co2	C21	98.96(5)	C14	C13	O3	117.88(11)
C25	Co2	C22	97.71(6)	C14	C13	C18	121.88(11)
C25	Co2	C24	96.05(5)	C18	C13	O3	120.20(11)
Co1	Co2A	Co3A	56.84(15)	C13	C14	C15	118.68(12)
Co4A	Co2A	Co1	57.76(15)	C16	C15	C14	120.44(12)
Co4A	Co2A	Co3A	60.59(18)	C15	C16	C17	119.95(12)
Co1	Co3	Co4	60.489(8)	C16	C17	C18	120.28(12)
Co2	Co3	Co1	60.284(8)	C13	C18	C17	118.75(12)
Co2	Co3	Co4	60.894(8)	Co1	C19	Co3	78.59(5)
C19	Co3	Co1	49.93(4)	O4	C19	Co1	143.29(10)
C19	Co3	Co2	110.09(4)	O4	C19	Co3	138.11(10)
C19	Co3	Co4	81.09(4)	O5	C20	Co1	174.00(11)
C23	Co3	Co1	109.40(4)	Co1	C21	Co2	78.66(4)
C23	Co3	Co2	110.82(4)	O6	C21	Co1	143.10(10)
C23	Co3	Co4	168.82(4)	O6	C21	Co2	138.21(10)
C23	Co3	C19	95.89(5)	O8	C22	Co2	178.30(12)
C23	Co3	C24	97.70(5)	O7	C23	Co3	179.28(12)
C24	Co3	Co1	110.92(3)	Co2	C24	Co3	78.29(4)
C24	Co3	Co2	50.73(3)	O9	C24	Co2	140.66(10)
C24	Co3	Co4	82.69(3)	O9	C24	Co3	141.01(10)
C24	Co3	C19	159.73(5)	O10	C25	Co2	177.10(11)
C29	Co3	Co1	138.48(4)	O11	C26	Co4	176.89(12)
C29	Co3	Co2	135.68(4)	O12	C27	Co4	179.02(13)
C29	Co3	Co4	92.38(4)	O13	C28	Co4	178.39(13)

Table S5 Bond Angles for mo_B1959_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C29	Co3	C19	98.45(5)	O14	C29	Co3	177.40(12)

Table S6 Torsion Angles for mo_B1959_0m.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Co1	P1	O1	C1	-173.05(9)	O3	C13	C18	C17	-178.23(11)
Co1	P1	O2	C7	-121.24(9)	C1	C2	C3	C4	0.2(2)
Co1	P1	O3	C13	-14.24(11)	C2	C1	C6	C5	0.40(19)
P1	O1	C1	C2	96.58(13)	C2	C3	C4	C5	0.8(2)
P1	O1	C1	C6	-87.70(13)	C3	C4	C5	C6	-1.2(2)
P1	O2	C7	C8	-75.43(15)	C4	C5	C6	C1	0.6(2)
P1	O2	C7	C12	108.66(14)	C6	C1	C2	C3	-0.8(2)
P1	O3	C13	C14	108.09(11)	C7	C8	C9	C10	0.1(2)
P1	O3	C13	C18	-74.37(13)	C8	C7	C12	C11	0.1(3)
O1	P1	O2	C7	120.20(10)	C8	C9	C10	C11	-0.5(2)
O1	P1	O3	C13	109.89(10)	C9	C10	C11	C12	0.7(3)
O1	C1	C2	C3	174.75(12)	C10	C11	C12	C7	-0.5(3)
O1	C1	C6	C5	-175.16(11)	C12	C7	C8	C9	0.1(2)
O2	P1	O1	C1	-48.64(10)	C13	C14	C15	C16	-1.02(19)
O2	P1	O3	C13	-145.59(10)	C14	C13	C18	C17	-0.79(19)
O2	C7	C8	C9	-175.67(12)	C14	C15	C16	C17	0.0(2)
O2	C7	C12	C11	175.95(16)	C15	C16	C17	C18	0.6(2)
O3	P1	O1	C1	54.06(11)	C16	C17	C18	C13	-0.3(2)
O3	P1	O2	C7	13.73(11)	C18	C13	C14	C15	1.42(18)
O3	C13	C14	C15	178.92(10)					

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for mo_B1959_0m.

Atom	*x*	*y*	*z*	U(eq)
H2	8933.03	5875.58	3338.51	36
H3	10583.32	7088.4	3326.27	48
H4	11940.56	6778.73	3959.79	49
H5	11689.95	5222.56	4601.38	44
H6	10037.03	4020.75	4625.99	32
H8	10422.29	2419.29	3505.87	35
H9	11602.75	824.84	3164.6	39
H10	10954.08	-977.87	2610.71	41
H11	9116.14	-1234.17	2402.26	60
H12	7923.71	356.31	2735.62	48

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for mo_B1959_0m.

Atom	*x*	*y*	*z*	U(eq)
H14	8739.9	-1310.59	4104.87	29
H15	8465.37	-2946.67	4732.44	34
H16	8287.49	-2024.32	5497.51	33
H17	8377.45	536.47	5641.5	35
H18	8619.07	2187.36	5013.5	31

Table S8 Atomic Occupancy for mo_B1959_0m.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
Co2	0.9630(4)	Co2A	0.0370(4)	Co3	0.9630(4)
Co3A	0.0370(4)	Co4	0.9630(4)	Co4A	0.0370(4)

Experimental

Single crystals of $C_{29}H_{15}Co_4O_{14}P$ **[mo_B1959_0m]** were **[]**. A suitable crystal was selected and **[]** on a **Bruker SMART APEX2 area detector** diffractometer. The crystal was kept at 100.0 K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the XL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

Crystal structure determination of [mo_B1959_0m]

Crystal Data for $C_{29}H_{15}Co_4O_{14}P$ (M =854.10 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 12.5987(10) Å, b = 8.9773(9) Å, c = 27.953(2) Å, β = 96.829(3)°, V = 3139.2(5) Å^3, Z = 4, T = 100.0 K, μ(MoKα) = 2.198 mm^{-1}, *Dcalc* = 1.807 g/cm^3, 80868 reflections measured (4.768° ≤ 2Θ ≤ 66.294°), 11958 unique (R_{int} = 0.0294, R_{sigma} = 0.0190) which were used in all calculations. The final R_1 was 0.0236 (I > 2σ(I)) and wR_2 was 0.0579 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
2. Others
 Sof(Co2A)=Sof(Co3A)=Sof(Co4A)=1-FVAR(1)
 Sof(Co2)=Sof(Co3)=Sof(Co4)=FVAR(1)
3.a Aromatic/amide H refined with riding coordinates:
 C2(H2), C3(H3), C4(H4), C5(H5), C6(H6), C8(H8), C9(H9), C10(H10), C11(H11),
 C12(H12), C14(H14), C15(H15), C16(H16), C17(H17), C18(H18)
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