

SUPPORTING INFORMATION

Table 1. Crystal data and structure refinement for 3.

Empirical formula	C ₂₅ H ₄₆ Cl ₂ Mo N ₃ O P Si ₂
Formula weight	658.64
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 9.7269(2) Å α = 90° b = 17.7600(4) Å β = 94.237(1)° c = 18.9629(4) Å γ = 90°
Volume, Z	3266.88(12) Å ³ , 4
Density (calculated)	1.339 Mg/m ³
Absorption coefficient	0.709 mm ⁻¹
F(000)	1376
Crystal size	0.28 x 0.16 x 0.14 mm
Theta range for data collection	2.10 to 27.50°
Limiting indices	-12 ≤ h ≤ 11, -21 ≤ k ≤ 22, -22 ≤ l ≤ 24
Reflections collected	21565
Independent reflections	7435 [R(int) = 0.0308]
Absorption correction	Empirical
Max. and min. transmission	0.928 and 0.712
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7435 / 0 / 461

Goodness-of-fit on F^2	1.027
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0283$, $wR_2 = 0.0676$ [6045]
R indices (all data)	$R_1 = 0.0409$, $wR_2 = 0.0734$
Extinction coefficient	0.0010(2)
Largest diff. peak and hole	0.492 and -0.702 $e.\text{\AA}^{-3}$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 3. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Mo	-76(1)	297(1)	2020(1)	20(1)
C11	-2353(1)	550(1)	2480(1)	29(1)
C12	237(1)	-797(1)	2816(1)	33(1)
P1	595(1)	926(1)	3310(1)	31(1)
Si1	-1285(1)	1875(1)	1139(1)	25(1)
Si2	3033(1)	-466(1)	1633(1)	26(1)
N1	43(2)	1341(1)	1611(1)	21(1)
N2	1936(2)	310(1)	1830(1)	22(1)
N3	-896(2)	-281(1)	1374(1)	23(1)
C1	1370(2)	1611(1)	1762(1)	22(1)
C2	2411(2)	1043(1)	1876(1)	23(1)
C3	3802(2)	1269(1)	2010(1)	29(1)
C4	4135(2)	2018(1)	2033(1)	34(1)
C5	3114(2)	2571(1)	1928(1)	34(1)
C6	1756(2)	2374(1)	1797(1)	26(1)
C7	-1742(2)	-839(1)	1074(1)	23(1)
C8	-1846(2)	-951(1)	341(1)	30(1)
C9	-2674(2)	-1520(1)	55(1)	35(1)
C10	-3390(2)	-1983(1)	483(1)	35(1)
C11	-3289(3)	-1871(1)	1209(1)	36(1)
C12	-2479(2)	-1300(1)	1508(1)	30(1)
C13	-2147(3)	2473(2)	1775(2)	37(1)
C14	-536(3)	2468(2)	449(2)	39(1)
C15	-2531(3)	1204(2)	695(2)	37(1)
C16	4026(3)	-766(2)	2463(1)	41(1)
C17	4219(3)	-178(2)	954(1)	35(1)
C18	1938(3)	-1252(1)	1276(2)	36(1)
C19	-248(3)	505(2)	4042(1)	44(1)
C20	2398(3)	881(3)	3626(2)	58(1)
C21	150(3)	1916(2)	3396(2)	47(1)
O1	4807(2)	1177(1)	4950(1)	42(1)
C22	6233(3)	1568(2)	4056(2)	65(1)
C23	6149(3)	1400(2)	4822(2)	58(1)
C24	4641(3)	965(2)	5660(1)	56(1)
C25	3177(4)	782(2)	5740(2)	77(1)

Table 3. Bond lengths [Å] and angles [deg] for 3.

Mo-N3	1.745(2)
Mo-N2	2.017(2)
Mo-N1	2.018(2)
Mo-Cl2	2.4640(5)
Mo-Cl1	2.4802(5)
Mo-P1	2.7241(6)
P1-C20	1.812(3)
P1-C21	1.821(3)
P1-C19	1.823(3)
Si1-N1	1.788(2)
Si1-C13	1.853(3)
Si1-C15	1.856(2)
Si1-C14	1.868(3)
Si2-N2	1.799(2)
Si2-C18	1.853(3)
Si2-C16	1.863(3)
Si2-C17	1.863(3)
N1-C1	1.386(2)
N2-C2	1.383(3)
N3-C7	1.384(2)
C1-C6	1.407(3)
C1-C2	1.434(3)
C2-C3	1.417(3)
C3-C4	1.369(3)
C3-H3	0.96(2)
C4-C5	1.400(3)
C4-H4	0.95(3)
C5-C6	1.371(3)
C5-H5	0.93(2)
C6-H6	0.87(2)
C7-C12	1.397(3)
C7-C8	1.400(3)
C8-C9	1.379(3)
C8-H8	0.93(3)
C9-C10	1.379(3)
C9-H9	0.89(2)
C10-C11	1.387(3)
C10-H10	0.88(3)
C11-C12	1.380(3)
C11-H11	0.96(3)
C12-H12	0.93(2)
C13-H13A	0.95(3)
C13-H13B	0.96(3)
C13-H13C	0.97(3)
C14-H14A	0.88(3)
C14-H14B	0.84(4)
C14-H14C	0.99(3)
C15-H15A	0.91(3)
C15-H15B	1.00(3)
C15-H15C	0.91(3)
C16-H16A	0.90(3)

C16-H16B	1.02 (3)
C16-H16C	0.95 (3)
C17-H17A	0.91 (4)
C17-H17B	0.93 (3)
C17-H17C	0.90 (4)
C18-H18A	0.97 (3)
C18-H18B	0.90 (3)
C18-H18C	0.94 (3)
C19-H19A	0.95 (3)
C19-H19B	0.87 (3)
C19-H19C	0.91 (3)
C20-H20A	1.01 (3)
C20-H20B	0.99 (3)
C20-H20C	1.00 (4)
C21-H21A	0.97 (3)
C21-H21B	1.02 (4)
C21-H21C	1.05 (3)
O1-C23	1.403 (3)
O1-C24	1.418 (3)
C22-C23	1.492 (4)
C22-H22A	0.9600
C22-H22B	0.9600
C22-H22C	0.9600
C23-H23A	0.9700
C23-H23B	0.9700
C24-C25	1.480 (4)
C24-H24A	0.9700
C24-H24B	0.9700
C25-H25A	0.9600
C25-H25B	0.9600
C25-H25C	0.9600
N3-Mo-N2	106.25 (7)
N3-Mo-N1	107.85 (7)
N2-Mo-N1	80.56 (6)
N3-Mo-C12	89.77 (5)
N2-Mo-C12	92.36 (5)
N1-Mo-C12	162.21 (5)
N3-Mo-C11	88.87 (6)
N2-Mo-C11	164.69 (5)
N1-Mo-C11	92.69 (5)
C12-Mo-C11	90.06 (2)
N3-Mo-P1	159.80 (6)
N2-Mo-P1	89.12 (5)
N1-Mo-P1	87.22 (5)
C12-Mo-P1	76.31 (2)
C11-Mo-P1	76.76 (2)
C20-P1-C21	104.1 (2)
C20-P1-C19	102.1 (2)
C21-P1-C19	101.82 (14)
C20-P1-Mo	116.14 (11)
C21-P1-Mo	115.68 (10)
C19-P1-Mo	115.05 (10)
N1-Si1-C13	108.80 (10)

N1-Si1-C15	108.08 (10)
C13-Si1-C15	110.57 (13)
N1-Si1-C14	110.14 (10)
C13-Si1-C14	110.57 (13)
C15-Si1-C14	108.66 (13)
N2-Si2-C18	108.60 (10)
N2-Si2-C16	108.80 (11)
C18-Si2-C16	110.02 (14)
N2-Si2-C17	109.85 (10)
C18-Si2-C17	108.82 (13)
C16-Si2-C17	110.72 (13)
C1-N1-Si1	123.21 (13)
C1-N1-Mo	108.49 (12)
Si1-N1-Mo	128.29 (8)
C2-N2-Si2	122.33 (13)
C2-N2-Mo	108.86 (12)
Si2-N2-Mo	128.81 (9)
C7-N3-Mo	159.6 (2)
N1-C1-C6	125.7 (2)
N1-C1-C2	115.1 (2)
C6-C1-C2	119.2 (2)
N2-C2-C3	126.0 (2)
N2-C2-C1	115.1 (2)
C3-C2-C1	118.9 (2)
C4-C3-C2	120.0 (2)
C4-C3-H3	121.0 (13)
C2-C3-H3	118.9 (13)
C3-C4-C5	120.9 (2)
C3-C4-H4	119 (2)
C5-C4-H4	120 (2)
C6-C5-C4	120.7 (2)
C6-C5-H5	121.7 (13)
C4-C5-H5	117.6 (13)
C5-C6-C1	120.3 (2)
C5-C6-H6	119.0 (14)
C1-C6-H6	120.7 (14)
N3-C7-C12	119.5 (2)
N3-C7-C8	120.5 (2)
C12-C7-C8	120.0 (2)
C9-C8-C7	119.4 (2)
C9-C8-H8	124 (2)
C7-C8-H8	117 (2)
C8-C9-C10	120.8 (2)
C8-C9-H9	117 (2)
C10-C9-H9	122 (2)
C9-C10-C11	119.8 (2)
C9-C10-H10	121 (2)
C11-C10-H10	119 (2)
C12-C11-C10	120.6 (2)
C12-C11-H11	120 (2)
C10-C11-H11	119 (2)
C11-C12-C7	119.4 (2)
C11-C12-H12	120.8 (14)
C7-C12-H12	119.8 (14)

Si1-C13-H13A	113 (2)
Si1-C13-H13B	111 (2)
H13A-C13-H13B	108 (2)
Si1-C13-H13C	111 (2)
H13A-C13-H13C	105 (2)
H13B-C13-H13C	109 (3)
Si1-C14-H14A	112 (2)
Si1-C14-H14B	109 (3)
H14A-C14-H14B	108 (3)
Si1-C14-H14C	112 (2)
H14A-C14-H14C	102 (3)
H14B-C14-H14C	115 (3)
Si1-C15-H15A	109 (2)
Si1-C15-H15B	112 (2)
H15A-C15-H15B	104 (2)
Si1-C15-H15C	112 (2)
H15A-C15-H15C	112 (3)
H15B-C15-H15C	108 (2)
Si2-C16-H16A	111 (2)
Si2-C16-H16B	107 (2)
H16A-C16-H16B	111 (3)
Si2-C16-H16C	111 (2)
H16A-C16-H16C	106 (3)
H16B-C16-H16C	111 (2)
Si2-C17-H17A	115 (2)
Si2-C17-H17B	107 (2)
H17A-C17-H17B	105 (3)
Si2-C17-H17C	113 (2)
H17A-C17-H17C	106 (3)
H17B-C17-H17C	110 (3)
Si2-C18-H18A	111 (2)
Si2-C18-H18B	113 (2)
H18A-C18-H18B	111 (2)
Si2-C18-H18C	109 (2)
H18A-C18-H18C	106 (2)
H18B-C18-H18C	107 (2)
P1-C19-H19A	114 (2)
P1-C19-H19B	110 (2)
H19A-C19-H19B	104 (3)
P1-C19-H19C	110 (2)
H19A-C19-H19C	113 (3)
H19B-C19-H19C	106 (3)
P1-C20-H20A	104 (2)
P1-C20-H20B	111 (2)
H20A-C20-H20B	108 (2)
P1-C20-H20C	112 (2)
H20A-C20-H20C	119 (3)
H20B-C20-H20C	103 (3)
P1-C21-H21A	108 (2)
P1-C21-H21B	106 (2)
H21A-C21-H21B	106 (2)
P1-C21-H21C	104 (2)
H21A-C21-H21C	116 (3)
H21B-C21-H21C	116 (3)

C23-O1-C24	114.3(2)
C23-C22-H22A	109.5
C23-C22-H22B	109.5
H22A-C22-H22B	109.5
C23-C22-H22C	109.5
H22A-C22-H22C	109.5
H22B-C22-H22C	109.5
O1-C23-C22	110.1(2)
O1-C23-H23A	109.6
C22-C23-H23A	109.6
O1-C23-H23B	109.6
C22-C23-H23B	109.6
H23A-C23-H23B	108.2
O1-C24-C25	109.4(2)
O1-C24-H24A	109.8
C25-C24-H24A	109.8
O1-C24-H24B	109.8
C25-C24-H24B	109.8
H24A-C24-H24B	108.2
C24-C25-H25A	109.5
C24-C25-H25B	109.5
H25A-C25-H25B	109.5
C24-C25-H25C	109.5
H25A-C25-H25C	109.5
H25B-C25-H25C	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for 3. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Mo	19(1)	20(1)	20(1)	1(1)	2(1)	-2(1)
C11	22(1)	36(1)	31(1)	0(1)	8(1)	-2(1)
C12	38(1)	28(1)	33(1)	10(1)	3(1)	1(1)
P1	28(1)	40(1)	24(1)	-1(1)	4(1)	-5(1)
Si1	22(1)	22(1)	30(1)	3(1)	2(1)	1(1)
Si2	24(1)	28(1)	27(1)	2(1)	2(1)	5(1)
N1	18(1)	22(1)	22(1)	-1(1)	4(1)	-1(1)
N2	20(1)	26(1)	22(1)	1(1)	2(1)	0(1)
N3	22(1)	22(1)	23(1)	1(1)	3(1)	0(1)
C1	23(1)	26(1)	17(1)	-2(1)	4(1)	-2(1)
C2	21(1)	30(1)	18(1)	-2(1)	6(1)	-2(1)
C3	21(1)	39(1)	28(1)	-4(1)	2(1)	-2(1)
C4	24(1)	43(1)	35(1)	-7(1)	5(1)	-11(1)
C5	38(1)	32(1)	33(1)	-7(1)	9(1)	-15(1)
C6	30(1)	25(1)	26(1)	-2(1)	7(1)	-3(1)
C7	23(1)	19(1)	28(1)	-2(1)	0(1)	1(1)
C8	30(1)	32(1)	29(1)	1(1)	5(1)	-4(1)
C9	40(1)	38(1)	26(1)	-8(1)	1(1)	-5(1)
C10	34(1)	29(1)	42(1)	-9(1)	-4(1)	-8(1)
C11	39(1)	33(1)	37(1)	2(1)	3(1)	-12(1)
C12	31(1)	31(1)	26(1)	1(1)	2(1)	-7(1)
C13	27(1)	34(1)	50(2)	-4(1)	8(1)	3(1)
C14	38(1)	38(2)	41(1)	14(1)	3(1)	3(1)
C15	37(1)	36(1)	37(1)	4(1)	-12(1)	-4(1)
C16	37(1)	47(2)	37(1)	9(1)	-2(1)	9(1)
C17	30(1)	40(2)	37(1)	-1(1)	10(1)	4(1)
C18	38(1)	29(1)	42(1)	-6(1)	7(1)	3(1)
C19	54(2)	52(2)	27(1)	3(1)	8(1)	-8(1)
C20	36(2)	106(3)	30(1)	-8(2)	-8(1)	-7(2)
C21	64(2)	43(2)	35(1)	-10(1)	16(1)	-12(1)
O1	39(1)	51(1)	36(1)	2(1)	-4(1)	-3(1)
C22	48(2)	74(2)	75(2)	1(2)	23(2)	11(2)
C23	35(1)	77(2)	62(2)	-11(2)	0(1)	5(1)
C24	71(2)	61(2)	34(1)	3(1)	-7(1)	1(2)
C25	102(3)	92(3)	39(2)	2(2)	12(2)	-48(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 3.

	x	y	z	U(eq)
H3	4500(2)	888(13)	2102(11)	25(6)
H4	5070(3)	2161(15)	2146(14)	50(8)
H5	3390(2)	3074(12)	1952(11)	23(5)
H6	1140(2)	2727(12)	1745(11)	21(6)
H8	-1370(3)	-610(15)	73(14)	42(7)
H9	-2730(2)	-1574(14)	-415(14)	39(7)
H10	-3910(3)	-2350(15)	304(14)	44(7)
H11	-3770(3)	-2209(15)	1504(14)	48(8)
H12	-2420(2)	-1218(13)	1996(13)	30(6)
H13A	-1540(3)	2834(16)	2003(15)	54(8)
H13B	-2920(3)	2736(17)	1540(16)	61(9)
H13C	-2480(3)	2173(19)	2153(17)	71(10)
H14A	-200(3)	2893(19)	628(17)	65(10)
H14B	110(4)	2230(2)	290(2)	96(14)
H14C	-1250(3)	2646(17)	91(16)	59(8)
H15A	-3170(3)	1467(16)	415(15)	53(8)
H15B	-2090(3)	865(16)	357(14)	47(8)
H15C	-2940(3)	909(17)	1013(17)	62(9)
H16A	4620(3)	-409(17)	2620(17)	59(9)
H16B	4530(3)	-1249(18)	2349(16)	67(9)
H16C	3430(3)	-846(16)	2828(16)	58(9)
H17A	4940(4)	120(2)	1119(18)	78(11)
H17B	4620(3)	-613(19)	791(17)	69(10)
H17C	3790(4)	70(2)	589(19)	79(11)
H18A	1370(3)	-1097(14)	860(14)	40(7)
H18B	1420(3)	-1451(16)	1600(15)	49(8)
H18C	2500(3)	-1639(16)	1129(15)	52(8)
H19A	-30(3)	750(16)	4482(16)	52(8)
H19B	50(3)	47(19)	4115(16)	58(9)
H19C	-1170(4)	463(17)	3931(17)	64(10)
H20A	2600(3)	327(15)	3667(15)	42(8)
H20B	2540(3)	1104(18)	4103(18)	68(9)
H20C	2990(4)	1200(2)	3340(2)	98(13)
H21A	430(3)	2074(16)	3872(16)	53(8)
H21B	760(4)	2206(19)	3077(18)	81(11)
H21C	-910(4)	1935(19)	3252(18)	81(11)
H22A	7155	1720	3974	97
H22B	5604	1966	3918	97
H22C	5996	1125	3783	97
H23A	6793	1001	4965	70
H23B	6400	1844	5100	70
H24A	4930	1375	5975	67
H24B	5213	530	5784	67
H25A	3065	638	6220	116
H25B	2899	373	5430	116

H25C

2617

1215

5621

116
