SUPPLEMENTARY MATERIAL

Table S1 - Crystal Data and Structure Refinement for 3.

Table S2 - Atomic coordinates ($x \ 10^4$) and equivalent isotropic displacement parameters (Å² x 10³) for 3.

Table S3 - Bond lengths (Å) and angles (degrees) for 3.

Table S4 - Anisotropic Displacement Parameters ($\mathring{A}^2 \times 10^3$) for 3.

Table S5 - Hydrogen coordinates ($x\;10^4$) and isotropic displacement parameters (Å $^2\;x\;10^3$) for 3.

Figure 1 - ORTEP drawing of 3.

Table S1' - Crystal Data and Structure Refinement for 8.

Table S2' - Atomic coordinates ($x \ 10^4$) and equivalent isotropic displacement parameters (Å² x 10^3) for 8.

Table S3' - Bond lengths (Å) and angles (degrees) for 8.

Table S4' - Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 8.

Table S5' - Hydrogen coordinates ($x \ 10^4$) and isotropic displacement parameters (Å² x 10^3) for 8.

Figure 1' - ORTEP drawing of 8.

Empirical formula	C ₃₀ H ₃₆ Nb O P S ₂ Si ₂
Formula weight	656.77
Temperature	250(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 17.063(8) Å.
	$b = 10.834(8) \text{ Å}$ $\beta = 108.76(4) \text{ deg.}$
	c = 18.488(6) Å.
Volume	3236(3) Å ³
Z, Calculated density	4, 1.348 g/cm^3
Absorption coefficient	6.46 cm^{-1}
Range of transmission factor	0.689-1.000
F(000)	1360
Crystal size	$0.4 \ge 0.3 \ge 0.3 \text{ mm}^3$
Theta range for data collection	2.21 to 28 deg.
Limiting indices	$-22 \le h \le 21, 0 \le k \le 14, 0 \le l \le 20$
Reflections collected / unique	7656 / 7413 [R(int) = 0.0914]
Completeness to theta $= 28.00$	94.8 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7413 / 0 / 334
Goodness-of-fit on F^2	0.958
Final R indices [I>2sigma(I)]	R1 = 0.0863, wR2 = 0.1398
R indices (all data)	R1 = 0.3249, wR2 = 0.2046
Largest diff. peak and hole	0.747 and -0.671 e.Å ⁻³

Table S1'. Crystal data and structure refinement for **3**.

	Х	У	Z	U(eq)
Nb(1)	7965(1)	2237(1)	8749(1)	54(1)
P(1)	8360(3)	265(4)	11459(3)	58(1)
S (1)	7644(2)	1186(4)	9851(3)	55(1)
S(2)	9470(3)	1378(4)	10723(3)	80(2)
Si(1)	7107(3)	-1016(4)	8030(3)	67(2)
Si(2)	6425(3)	4542(4)	9214(3)	72(2)
O(1)	6089(7)	2108(10)	7722(6)	73(4)
C(1)	6783(9)	2126(15)	8153(9)	55(5)
C(2)	8493(8)	1001(13)	10624(9)	52(4)
C(3)	7906(11)	228(14)	8235(12)	65(6)
C(4)	7979(11)	1126(14)	7673(10)	62(5)
C(5)	8728(12)	1721(16)	7919(14)	77(6)
C(6)	9149(10)	1228(17)	8609(14)	78(6)
C(7)	8667(12)	309(15)	8788(11)	63(5)
C(8)	7743(12)	-2447(16)	8347(13)	124(9)
C(9)	6557(13)	-1020(20)	6979(11)	132(9)
C(10)	6328(9)	-892(14)	8550(10)	77(6)
C(11)	7435(9)	4107(12)	9092(11)	52(5)
C(12)	8182(10)	3890(13)	9665(9)	61(5)
C(13)	8857(11)	3906(13)	9422(13)	68(6)
C(14)	8546(12)	4227(14)	8616(13)	69(6)
C(15)	7674(12)	4328(13)	8397(11)	68(6)
C(16)	5884(10)	3313(17)	9525(16)	147(11)
C(17)	6609(12)	5839(19)	9866(14)	129(9)
C(18)	5739(12)	5132(19)	8251(13)	135(9)
C(19)	7255(8)	64(13)	11226(9)	48(4)
C(20)	6820(10)	-1013(15)	10958(10)	69(5)
C(21)	5987(12)	-1120(17)	10801(12)	85(7)
C(22)	5571(11)	-160(20)	10912(12)	81(7)
C(23)	5927(12)	930(20)	11203(11)	86(7)
C(24)	6780(11)	989(14)	11340(11)	78(6)
C(25)	8708(8)	-1320(15)	11383(10)	52(5)
C(26)	9085(10)	-1950(20)	12064(10)	71(6)
C(27)	9323(11)	-3190(20)	12049(15)	90(8)
C(28)	9167(13)	-3726(19)	11298(18)	93(8)
C(29)	8854(12)	-3086(18)	10684(12)	71(6)
C(30)	8578(10)	-1913(15)	10684(11)	65(6)

Table S2'. Atomic coordinates ($x \ 10^4$) and equivalent isotropic displacement parameters (Å² x 10³) for **3**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

$T_{a(1)}-N(1)$	2 327(5)
Ta(1)-Cl(3)	2.393(2)
Ta(1)-Cl(2)	2.407(2)
Ta(1)-Cl(1)	2.407(2)
Ta(1)-C(14)	2.431(8)
Ta(1)-C(11)	2.447(7)
Ta(1)-S(1)	2.4558(19)
Ta(1)-C(13)	2.463(8)
Ta(1)-C(10)	2.472(8)
Ta(1)-C(12)	2.484(7)
S(1)-C(1)	1.734(7)
N(1)-C(1)	1.337(7)
N(1)-C(4)	1.352(8)
N(2)-C(1)	1.328(9)
N(2)-C(2)	1.340(9)
C(2)-C(3)	1.402(10)
C(2)-C(6)	1.486(11)
C(3)-C(4)	1.349(10)
C(4)-C(5)	1.530(10)
C(10)-C(14)	1.390(14)
C(10)-C(11)	1.401(13)
C(10)-C(15)	1.485(13)
C(11)-C(12)	1.411(10)
C(11)-C(16)	1.531(11)
C(12)-C(13)	1.429(10)
C(12)-C(17)	1.469(11)
C(13)-C(14)	1.399(14)
C(13)-C(18)	1.476(11)
C(14)-C(19)	1.516(13)
N(1)-Ta(1)-Cl(3)	87.65(13)
N(1)-Ta(1)-Cl(2)	76.30(16)
CI(3)-Ta(1)-CI(2)	85.54(11)
N(1)-Ta(1)-Cl(1)	76.24(15)
CI(3)-Ta(1)- $CI(1)$	85.41(10)
CI(2)-Ta(1)-CI(1)	151.37(8)
N(1)-Ta(1)-C(14)	159.0(3)
CI(3)-Ta(1)-C(14)	83.2(3)
CI(2)-Ia(1)-C(14)	121.6(3)
CI(1)-Ia(1)-C(14)	84.2(3)
N(1)-1a(1)-C(11)	138.2(2)
$C_1(3) - Ta(1) - C(11)$	100 2(2)
$C_1(2)$ -Ta(1)- $C_1(1)$	100.3(2) 105.5(2)
$C(14) T_0(1) C(11)$	103.3(2) 54.7(2)
U(14) - 1a(1) - U(11) $N(1) T_0(1) S(1)$	34.7(3) 64.21(12)
11(1) - 1a(1) - 3(1)	04.31(12)

 Table S3'. Bond lengths [Å] and angles [deg] for 3.

Cl(3)-Ta(1)-S(1)	151.96(7)
Cl(2)-Ta(1)-S(1)	87.49(9)
Cl(1)-Ta(1)-S(1)	87.87(8)
C(14)-Ta(1)-S(1)	123.1(3)
C(11)-Ta(1)-S(1)	74.00(19)
N(1)-Ta(1)-C(13)	160.9(2)
Cl(3)-Ta(1)-C(13)	79.73(17)
Cl(2)-Ta(1)-C(13)	88.4(2)
Cl(1)-Ta(1)-C(13)	116.6(2)
C(14)-Ta(1)-C(13)	33.2(3)
C(11)-Ta(1)-C(13)	55.2(2)
S(1)-Ta(1)-C(13)	127.20(17)
N(1)-Ta(1)-C(10)	144.0(3)
Cl(3)-Ta(1)-C(10)	114.5(3)
Cl(2)-Ta(1)-C(10)	130.6(2)
Cl(1)-Ta(1)-C(10)	77.7(2)
C(14)-Ta(1)-C(10)	32.9(3)
C(11)-Ta(1)-C(10)	33.1(3)
S(1)-Ta(1)-C(10)	90.4(3)
C(13)-Ta(1)-C(10)	55.2(3)
N(1)-Ta(1)-C(12)	145.8(2)
Cl(3)-Ta(1)-C(12)	109.44(17)
Cl(2)-Ta(1)-C(12)	75.81(17)
Cl(1)-Ta(1)-C(12)	132.77(17)
C(14)-Ta(1)-C(12)	55.2(3)
C(11)-Ta(1)-C(12)	33.2(2)
S(1)-Ta(1)-C(12)	95.03(17)
C(13)-Ta(1)-C(12)	33.6(2)
C(10)-Ta(1)-C(12)	55.2(3)
C(1)-S(1)-Ta(1)	84.6(2)
C(1)-N(1)-C(4)	116.6(6)
C(1)-N(1)-Ta(1)	99.5(4)
C(4)-N(1)-Ta(1)	143.8(4)
C(1)-N(2)-C(2)	116.2(6)
N(2)-C(1)-N(1)	127.0(6)
N(2)-C(1)-S(1)	121.5(5)
N(1)-C(1)-S(1)	111.5(5)
N(2)-C(2)-C(3)	120.0(6)
N(2)-C(2)-C(6)	117.3(7)
C(3)-C(2)-C(6)	122.6(7)
C(4)-C(3)-C(2)	120.0(6)
C(3)-C(4)-N(1)	120.0(6)
C(3)-C(4)-C(5)	119.9(7)
N(1)-C(4)-C(5)	120.1(7)
C(14)-C(10)-C(11)	106.8(7)
C(14)-C(10)-C(15)	130.1(13)
C(11)-C(10)-C(15)	122.9(13)

C(14)-C(10)-Ta(1)	71.9(5)
C(11)-C(10)-Ta(1)	72.5(4)
C(15)-C(10)-Ta(1)	125.0(6)
C(10)-C(11)-C(12)	109.6(7)
C(10)-C(11)-C(16)	125.4(9)
C(12)-C(11)-C(16)	122.7(9)
C(10)-C(11)-Ta(1)	74.4(4)
C(12)-C(11)-Ta(1)	74.8(4)
C(16)-C(11)-Ta(1)	131.1(6)
C(11)-C(12)-C(13)	106.4(7)
C(11)-C(12)-C(17)	127.8(7)
C(13)-C(12)-C(17)	124.9(8)
C(11)-C(12)-Ta(1)	72.0(4)
C(13)-C(12)-Ta(1)	72.4(4)
C(17)-C(12)-Ta(1)	128.9(5)
C(14)-C(13)-C(12)	107.1(7)
C(14)-C(13)-C(18)	128.6(10)
C(12)-C(13)-C(18)	123.9(9)
C(14)-C(13)-Ta(1)	72.1(5)
C(12)-C(13)-Ta(1)	74.0(4)
C(18)-C(13)-Ta(1)	124.8(6)
C(10)-C(14)-C(13)	110.0(7)
C(10)-C(14)-C(19)	125.7(12)
C(13)-C(14)-C(19)	123.9(12)
C(10)-C(14)-Ta(1)	75.1(5)
C(13)-C(14)-Ta(1)	74.7(5)
C(19)-C(14)-Ta(1)	122.4(7)

	U11	U22	U33	U23	U13	U12
Nb(1)	54(1)	47(1)	65(1)	-4(1)	24(1)	-2(1)
P(1)	65(3)	62(3)	43(4)	-2(3)	12(3)	3(2)
S (1)	56(3)	62(3)	41(3)	-5(3)	10(3)	3(2)
S(2)	55(3)	92(4)	80(4)	13(3)	6(3)	-6(3)
Si(1)	86(4)	54(3)	66(5)	-22(3)	33(4)	-6(3)
Si(2)	59(3)	68(3)	88(5)	-24(4)	22(3)	2(3)
O(1)	86(8)	66(7)	40(8)	-1(7)	-21(7)	3(8)
C(1)	47(9)	74(11)	37(12)	1(11)	4(9)	-7(10)
C(2)	43(9)	77(11)	35(12)	11(10)	13(9)	17(8)
C(3)	83(14)	57(11)	74(17)	14(11)	51(13)	13(10)
C(4)	96(14)	43(9)	54(14)	19(10)	34(12)	35(10)
C(5)	69(14)	76(13)	100(20)	5(13)	49(14)	-19(10)
C(6)	56(12)	79(13)	110(20)	-6(15)	44(14)	2(11)
C(7)	73(13)	66(12)	66(16)	0(12)	43(13)	-3(11)
C(8)	147(17)	90(14)	200(30)	11(15)	150(20)	-13(13)
C(9)	150(20)	190(20)	38(15)	-28(16)	1(15)	-49(17)
C(10)	74(12)	81(12)	82(16)	-36(12)	36(12)	-22(10)
C(11)	47(10)	36(8)	62(14)	-6(9)	1(10)	-11(7)
C(12)	49(10)	55(10)	41(13)	-6(10)	-40(10)	13(9)
C(13)	76(13)	33(9)	110(20)	-7(12)	57(15)	-1(9)
C(14)	86(15)	39(10)	94(19)	-11(12)	42(15)	-20(10)
C(15)	88(15)	39(9)	61(16)	-9(10)	3(12)	-22(9)
C(16)	66(12)	109(15)	310(40)	21(19)	120(19)	-3(11)
C(17)	104(16)	132(18)	140(20)	-59(18)	27(16)	-5(14)
C(18)	100(16)	135(18)	120(20)	-3(17)	-33(16)	16(14)
C(19)	45(10)	56(9)	36(12)	-10(9)	6(9)	6(8)
C(20)	65(12)	79(12)	57(15)	19(11)	11(11)	-21(10)
C(21)	74(13)	83(13)	110(20)	13(14)	45(14)	-19(12)
C(22)	69(14)	115(18)	44(16)	-8(15)	-2(12)	-12(13)
C(23)	72(14)	150(19)	43(15)	4(15)	26(12)	55(14)
C(24)	87(14)	65(11)	76(17)	-8(12)	19(13)	15(11)
C(25)	26(8)	101(13)	16(11)	-16(11)	-13(8)	-10(9)
C(26)	41(10)	150(20)	23(13)	5(14)	9(10)	-21(11)
C(27)	65(13)	88(16)	110(20)	68(15)	13(15)	15(12)
C(28)	72(15)	72(15)	130(30)	-45(17)	33(18)	-36(12)
C(29)	69(13)	87(17)	54(17)	-4(12)	15(12)	-12(11)
C(30)	55(11)	66(13)	52(15)	-12(11)	-15(10)	8(9)

Table S4'. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: -2 π^2 [$h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12$]

	X	у	Z	U(eq)
H(4)	7571	1277	7208	74
H(5)	8911	2339	7663	92
H(6)	9676	1464	8915	93
H(7)	8838	-181	9224	76
H(8A)	7383	-3148	8285	185
H(8B)	8070	-2367	8875	185
H(8C)	8100	-2558	8044	185
H(9A)	6121	-1621	6860	198
H(9B)	6941	-1220	6715	198
H(9C)	6326	-216	6822	198
H(10A)	5959	-1587	8422	115
H(10B)	6016	-144	8403	115
H(10C)	6610	-883	9091	115
H(12)	8218	3746	10171	74
H(13)	9404	3744	9711	82
H(14)	8866	4346	8298	83
H(15)	7318	4501	7909	81
H(16A)	5798	2633	9175	221
H(16B)	5359	3613	9537	221
H(16C)	6210	3045	10026	221
H(17A)	6900	6475	9694	194
H(17B)	6935	5574	10368	194
H(17C)	6089	6157	9881	194
H(18A)	5638	4477	7882	203
H(18B)	6010	5803	8089	203
H(18C)	5222	5412	8294	203
H(20)	7113	-1697	10882	83
H(21)	5718	-1858	10618	102
H(22)	5000	-233	10785	97
H(23)	5626	1583	11303	103
H(24)	7042	1731	11526	94
H(26)	9181	-1548	12530	85
H(27)	9564	-3645	12494	108
H(28)	9296	-4552	11257	111
H(29)	8817	-3447	10217	85
H(30)	8307	-1511	10227	78

Table S5'. Hydrogen coordinates ($x \ 10^4$) and isotropic displacement parameters (Å² x 10³) for **3**.

Figure 1 - ORTEP drawing of 3.



Empirical formula	C ₂₉ H ₃₆ I ₄ Nb O P Si ₂
Formula weight	1088.24
Temperature	230(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	$a = 11.6080(10)$ Å, $\alpha = 81.77(2)$ deg.
	b = 12.194(5) Å, β = 78.420(10) deg.
	$c = 14.197(2)$ Å, $\gamma = 72.220(10)$ deg.
Volume	1867.4(8) Å ³
Z, Calculated density	2, 1.935 g/cm ³
Absorption coefficient	37.56cm ⁻¹
Range of transmisión factor	0.591-1.000
F(000)	1028
Crystal size	$0.3 \ge 0.3 \ge 0.2 \text{ mm}^3$
Theta range for data collection	2.17 to 27.99 deg.
Limiting indices	$-15 \le h \le 15, -15 \le k \le 16, 0 \le l \le 18$
Reflections collected / unique	9343 / 8989 [R(int) = 0.0218]
Completeness to theta $= 27.99$	99.7 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8989 / 0 / 343
Goodness-of-fit on F^2	1.027
Final R indices $[I > 2\sigma(I)]$	R1 = 0.0548, $wR2 = 0.1484$
R indices (all data)	R1 = 0.0672, $wR2 = 0.1576$
Largest diff. peak and hole	4.118 and -4.117 e.Å ⁻³

 Table S1. Crystal data and structure refinement for 8.

	X	v	Z	U(eq)
Nb(1)	3159(1)	7391(1)	2665(1)	29(1)
I(1)	5221(1)	4137(1)	1658(1)	46(1)
I(2)	-2089(1)	11099(1)	1332(1)	117(1)
I(3)	-1964(1)	8677(1)	1929(1)	72(1)
I(4)	-1817(1)	6266(1)	2611(1)	70(1)
P(1)	3158(1)	5454(1)	2158(1)	33(1)
Si(1)	3267(2)	10627(2)	1826(2)	58(1)
Si(2)	2574(2)	8182(2)	5349(1)	54(1)
O(1)	5036(4)	5960(4)	4075(4)	55(1)
C(1)	4377(5)	6449(5)	3569(4)	39(1)
C(11)	3747(6)	9019(5)	1765(4)	41(1)
C(12)	4800(5)	8215(5)	2103(5)	42(1)
C(13)	5078(5)	7162(5)	1653(5)	43(1)
C(14)	4236(6)	7316(5)	1034(4)	42(1)
C(15)	3416(6)	8436(5)	1096(4)	43(1)
C(16)	3604(12)	10981(9)	2946(9)	95(3)
C(17)	1640(10)	11254(8)	1651(9)	89(3)
C(18)	4287(12)	11148(7)	790(9)	104(4)
C(21)	2084(5)	7986(5)	4210(4)	37(1)
C(22)	1751(5)	7005(5)	4015(4)	39(1)
C(23)	1085(5)	7335(6)	3230(5)	44(1)
C(24)	1035(5)	8487(6)	2909(5)	43(1)
C(25)	1635(5)	8882(5)	3501(4)	38(1)
C(26)	1306(13)	9381(13)	5879(9)	135(7)
C(27)	4030(11)	8572(11)	5139(9)	96(3)
C(28)	2717(11)	6802(11)	6137(8)	92(3)
C(31)	2536(5)	4517(5)	3109(4)	39(1)
C(32)	3151(6)	4037(6)	3886(5)	48(1)
C(33)	2630(8)	3432(7)	4662(5)	61(2)
C(34)	1473(9)	3304(9)	4673(6)	74(2)
C(35)	877(7)	3759(9)	3903(7)	72(2)
C(36)	1392(6)	4389(7)	3119(5)	53(2)
C(41)	2403(5)	5467(5)	1151(4)	37(1)
C(42)	2547(7)	4454(6)	728(5)	50(2)
C(43)	1964(7)	4486(7)	-35(6)	58(2)
C(44)	1216(7)	5512(8)	-373(5)	58(2)
C(45)	1046(8)	6512(6)	47(6)	58(2)
C(46)	1644(7)	6493(5)	799(5)	47(1)

Table S2. Atomic coordinates ($x \ 10^4$) and equivalent isotropic displacement parameters (Å² x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Nb(1)-C(1)	2.069(6)
Nb(1)-C(22)	2.349(5)
Nb(1)-C(13)	2.356(5)
Nb(1)-C(12)	2 368(5)
Nb(1) - C(25)	2.300(3) 2 379(5)
Nb(1) - C(23)	2.377(5)
NU(1)-C(21)	2.307(3)
ND(1)-C(23)	2.399(0)
ND(1)-C(14)	2.401(6)
Nb(1)-C(24)	2.401(6)
Nb(1)-C(11)	2.407(6)
Nb(1)-C(15)	2.414(6)
Nb(1)-P(1)	2.5652(17)
I(1)-P(1)	2.4724(15)
I(2)-I(3)	2.9212(17)
I(3)-I(4)	2.9241(15)
P(1)-C(41)	1.817(6)
P(1)-C(31)	1.823(6)
Si(1)-C(16)	1 849(12)
Si(1) - C(18)	1 860(9)
Si(1) - C(17)	1.861(11)
$S_{i}(1) = C(11)$	1.877(6)
Si(1) - C(11) Si(2) - C(27)	1.877(0) 1.850(12)
SI(2) - C(27) Si(2) - C(26)	1.030(12) 1.951(10)
SI(2) - C(20)	1.651(10)
S1(2)-C(28)	1.805(11)
$S_1(2)$ - $C_2(21)$	1.88/(6)
O(1)-C(1)	1.131(7)
C(11)-C(12)	1.434(9)
C(11)-C(15)	1.435(9)
C(12)-C(13)	1.435(8)
C(13)-C(14)	1.396(9)
C(14)-C(15)	1.409(9)
C(21)-C(25)	1.424(8)
C(21)-C(22)	1.441(8)
C(22)-C(23)	1.424(9)
C(23)-C(24)	1.401(9)
C(24)-C(25)	1.407(9)
C(31)-C(36)	1.380(9)
C(31)-C(32)	1 394(9)
C(32)- $C(33)$	1.377(10)
C(32) = C(33) C(33) = C(34)	1.377(10) 1 305(13)
C(34) = C(35)	1.373(13) 1.270(14)
C(34)-C(33)	1.370(14) 1.208(10)
C(33)-C(30)	1.398(10)
C(41) - C(40)	1.384(9)
C(41)-C(42)	1.401(8)
C(42)-C(43)	1.377(10)
C(43)-C(44)	1.372(12)
C(44)-C(45)	1.378(11)
C(45)-C(46)	1.379(10)

 Table S3.
 Bond lengths [Å] and angles [deg] for 8.

C(1)-Nb(1)-C(22)	80.8(2)
C(1)-Nb(1)-C(13)	77.2(2)
C(22)-Nb(1)-C(13)	157.0(2)
C(1)-Nb(1)-C(12)	79.8(2)
C(22)-Nb(1)-C(12)	145.2(2)
C(13)-Nb(1)-C(12)	35.4(2)
C(1)-Nb(1)-C(25)	109.5(2)
C(22)-Nb(1)-C(25)	57.4(2)
C(13)-Nb(1)-C(25)	137.7(2)
C(12)-Nb(1)-C(25)	103.1(2)
C(1)-Nb(1)-C(21)	77.8(2)
C(22)-Nb(1)-C(21)	35.4(2)
C(13)-Nb(1)-C(21)	141.9(2)
C(12)-Nb(1)-C(21)	111.6(2)
C(25)-Nb(1)-C(21)	34.8(2)
C(1)-Nb(1)-C(23)	114.0(2)
C(22)-Nb(1)-C(23)	34.9(2)
C(13)-Nb(1)-C(23)	159.7(2)
C(12)-Nb(1)-C(23)	157.8(2)
C(25)-Nb(1)-C(23)	56.8(2)
C(21)-Nb(1)-C(23)	58.3(2)
C(1)-Nb(1)-C(14)	108.2(2)
C(22)-Nb(1)-C(14)	157.3(2)
C(13)-Nb(1)-C(14)	34.1(2)
C(12)-Nb(1)-C(14)	57.4(2)
C(25)-Nb(1)-C(14)	132.8(2)
C(21)-Nb(1)-C(14)	164.9(2)
C(23)-Nb(1)-C(14)	127.3(2)
C(1)-Nb(1)-C(24)	134.5(2)
C(22)-Nb(1)-C(24)	57.5(2)
C(13)-Nb(1)-C(24)	145.6(2)
C(12)-Nb(1)-C(24)	124.1(2)
C(25)-Nb(1)-C(24)	34.2(2)
C(21)-Nb(1)-C(24)	58.0(2)
C(23)-Nb(1)-C(24)	33.9(2)
C(14)-Nb(1)-C(24)	117.3(2)
C(1)-Nb(1)-C(11)	113.0(2)
C(22)-Nb(1)-C(11)	139.1(2)
C(13)-Nb(1)-C(11)	58.4(2)
C(12)-Nb(1)-C(11)	34.9(2)
C(25)-Nb(1)-C(11)	81.8(2)
C(21)-Nb(1)-C(11)	107.3(2)
C(23)-Nb(1)-C(11)	125.0(2)
C(14)-Nb(1)-C(11)	57.6(2)
C(24)-Nb(1)- $C(11)$	91.5(2)
C(1)-IND (1) - $C(15)$	135.0(2)
U(22)-ND(1)- $U(15)$	145.8(2)
C(13)-IND (1) - $C(13)$	51.0(2)
C(12)-ND(1)- $C(15)$	57.2(2)

C(25)-Nb(1)-C(15)	98.8(2)
C(21)-Nb(1)-C(15)	132.5(2)
C(23)-Nb(1)-C(15)	112.8(2)
C(14)-Nb(1)-C(15)	34.0(2)
C(24)-Nb(1)-C(15)	88.8(2)
C(11)-Nb(1)-C(15)	34.6(2)
C(1)-Nb(1)-P(1)	87.33(17)
C(22)-Nb(1)-P(1)	84.78(15)
C(13)-Nb(1)-P(1)	87.40(15)
C(12)-Nb(1)-P(1)	122.74(15)
C(25)-Nb(1)-P(1)	133.56(15)
C(21)-Nb(1)-P(1)	119.62(15)
C(23)-Nb(1)-P(1)	76.78(15)
C(14)-Nb(1)-P(1)	75.06(14)
C(24)-Nb(1)-P(1)	104.32(16)
C(11)-Nb(1)-P(1)	132.04(15)
C(15)-Nb(1)-P(1)	99.73(15)
I(2)-I(3)-I(4)	177.39(3)
C(41)-P(1)-C(31)	104.1(3)
C(41)-P(1)-I(1)	101.6(2)
C(31)-P(1)-I(1)	99.90(19)
C(41)-P(1)-Nb(1)	118.61(19)
C(31)-P(1)-Nb(1)	115.55(19)
I(1)-P(1)-Nb(1)	114.55(6)
C(16)-Si(1)-C(18)	107.8(6)
C(16)-Si(1)-C(17)	114.4(6)
C(18)-Si(1)-C(17)	109.6(6)
C(16)-Si(1)-C(11)	110.4(4)
C(18)-Si(1)-C(11)	103.9(3)
C(17)-Si(1)-C(11)	110.2(4)
C(27)-Si(2)-C(26)	109.5(7)
C(27)-Si(2)-C(28)	110.0(6)
C(26)-Si(2)-C(28)	111.8(7)
C(27)-Si(2)-C(21)	113.9(4)
C(26)-Si(2)-C(21)	104.1(4)
C(28)-Si(2)-C(21)	107.4(4)
O(1)-C(1)-Nb(1)	178.2(5)
C(12)-C(11)-C(15)	105.9(5)
C(12)-C(11)-Si(1)	125.8(4)
C(15)-C(11)-Si(1)	125.0(5)
C(12)-C(11)-Nb(1)	71.0(3)
C(15)-C(11)-Nb(1)	73.0(3)
Si(1)-C(11)-Nb(1)	136.8(3)
C(11)-C(12)-C(13)	108.3(5)
C(11)-C(12)-Nb(1)	74.0(3)
C(13)-C(12)-Nb(1)	71.9(3)
C(14)-C(13)-C(12)	108.0(6)
C(14)-C(13)-Nb(1)	74.7(3)
C(12)-C(13)-Nb(1)	72.8(3)
C(13)-C(14)-C(15)	108.6(5)

C(1	3)-C(14)-Nb(1)	71.2(3)
C(1	5)-C(14)-Nb(1)	73.5(3)
C(1	4)-C(15)-C(11)	109.1(6)
C(1-	4)-C(15)-Nb(1)	72.5(3)
C(1	1)-C(15)-Nb(1)	72.4(3)
C(2	5)-C(21)-C(22)	105.0(5)
C(2	5)-C(21)-Si(2)	125.9(4)
C(2	2)-C(21)-Si(2)	126.9(5)
C(2	5)-C(21)-Nb(1)	72.3(3)
C(2	2)-C(21)-Nb(1)	70.9(3)
Si(2	2)-C(21)-Nb(1)	134.1(3)
C(2	3)-C(22)-C(21)	109.0(5)
C(2	3)-C(22)-Nb(1)	74.5(3)
C(2	1)-C(22)-Nb(1)	73.7(3)
C(2	4)-C(23)-C(22)	107.8(5)
C(2	4)-C(23)-Nb(1)	73.1(3)
C(2	2)-C(23)-Nb(1)	70.6(3)
C(2	3)-C(24)-C(25)	108.0(5)
C(2	3)-C(24)-Nb(1)	73.0(3)
C(2	5)-C(24)-Nb(1)	72.0(3)
C(2	4)-C(25)-C(21)	110.2(5)
C(2	4)-C(25)-Nb(1)	73.7(3)
C(2	1)-C(25)-Nb(1)	72.9(3)
C(3	6)-C(31)-C(32)	119.8(6)
C(3	6)-C(31)-P(1)	120.1(5)
C(3	2)-C(31)-P(1)	119.7(5)
C(3	3)-C(32)-C(31)	120.6(7)
C(3	2)-C(33)-C(34)	119.7(7)
C(3	5)-C(34)-C(33)	119.8(7)
C(3-	4)-C(35)-C(36)	120.9(8)
C(3	1)-C(36)-C(35)	119.3(7)
C(4	6)-C(41)-C(42)	118.5(6)
C(4	6)-C(41)-P(1)	119.9(4)
C(4	2)-C(41)-P(1)	121.6(5)
C(4	3)-C(42)-C(41)	120.5(6)
C(4	4)-C(43)-C(42)	120.0(7)
C(4	3)-C(44)-C(45)	120.1(6)
C(4	4)-C(45)-C(46)	120.2(7)
C(4	5)-C(46)-C(41)	120.5(6)

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: -2 π^2 [$h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12$]

	U11	U22	U33	U23	U13	U12
Nb(1)	29(1)	28(1)	31(1)	-3(1)	-1(1)	-11(1)
I(1)	43(1)	41(1)	51(1)	-10(1)	-3(1)	-5(1)
I(2)	166(1)	117(1)	93(1)	24(1)	-63(1)	-68(1)
I(3)	55(1)	108(1)	62(1)	-3(1)	-19(1)	-34(1)
I(4)	61(1)	88(1)	61(1)	-13(1)	-16(1)	-16(1)
P(1)	36(1)	29(1)	34(1)	-2(1)	-3(1)	-13(1)
Si(1)	71(1)	31(1)	66(1)	-4(1)	11(1)	-21(1)
Si(2)	53(1)	59(1)	43(1)	-17(1)	-14(1)	4(1)
O(1)	46(2)	56(3)	55(3)	4(2)	-15(2)	-4(2)
C(1)	35(3)	37(3)	42(3)	-3(2)	-1(2)	-11(2)
C(11)	49(3)	34(3)	43(3)	1(2)	0(2)	-22(2)
C(12)	40(3)	41(3)	48(3)	-5(2)	2(2)	-24(2)
C(13)	37(3)	43(3)	46(3)	-9(3)	11(2)	-16(2)
C(14)	54(3)	39(3)	35(3)	-6(2)	10(2)	-24(3)
C(15)	55(3)	40(3)	37(3)	3(2)	-4(2)	-23(3)
C(16)	131(10)	69(6)	98(8)	-29(6)	-10(7)	-44(6)
C(17)	82(6)	58(5)	106(8)	23(5)	-12(6)	-5(4)
C(18)	126(9)	36(4)	119(9)	3(5)	51(7)	-29(5)
C(21)	34(2)	38(3)	36(3)	-9(2)	1(2)	-7(2)
C(22)	35(3)	40(3)	37(3)	-5(2)	7(2)	-11(2)
C(23)	31(3)	53(3)	53(3)	-16(3)	1(2)	-17(2)
C(24)	33(3)	47(3)	43(3)	-9(3)	-6(2)	-1(2)
C(25)	34(2)	33(3)	41(3)	-4(2)	0(2)	-5(2)
C(26)	122(9)	147(11)	98(8)	-83(8)	-59(7)	73(9)
C(27)	94(7)	113(9)	103(8)	-30(7)	-41(6)	-38(7)
C(28)	107(8)	101(8)	65(6)	16(5)	-34(6)	-23(6)
C(31)	45(3)	30(3)	40(3)	-2(2)	1(2)	-15(2)
C(32)	53(3)	44(3)	45(3)	2(3)	-9(3)	-15(3)
C(33)	74(5)	62(4)	41(4)	9(3)	-2(3)	-20(4)
C(34)	72(5)	83(6)	52(4)	15(4)	16(4)	-25(4)
C(35)	47(4)	89(6)	75(6)	9(5)	6(4)	-31(4)
C(36)	47(3)	59(4)	52(4)	8(3)	-4(3)	-24(3)
C(41)	41(3)	36(3)	37(3)	0(2)	-5(2)	-18(2)
C(42)	60(4)	38(3)	55(4)	-8(3)	-12(3)	-15(3)
C(43)	66(4)	62(4)	57(4)	-22(3)	-10(3)	-25(4)
C(44)	64(4)	77(5)	46(4)	-1(3)	-18(3)	-34(4)
C(45)	69(4)	48(4)	65(5)	7(3)	-29(4)	-20(3)
C(46)	62(4)	35(3)	50(4)	3(3)	-19(3)	-19(3)

	Х	у	Z	U(eq)
H(12)	5230	8352	2540	50
H(13)	5708	6494	1757	52
H(14)	4220	6771	645	50
H(15)	2765	8748	758	52
H(16A)	4455	10625	2986	142
H(16B)	3107	10698	3494	142
H(16C)	3424	11804	2940	142
H(17A)	1539	11035	1056	133
H(17B)	1425	12081	1629	133
H(17C)	1117	10969	2178	133
H(18A)	4135	10967	198	156
H(18B)	5128	10776	855	156
H(18C)	4123	11969	782	156
H(22)	1941	6276	4347	47
H(23)	744	6868	2976	53
H(24)	669	8915	2395	51
H(25)	1725	9623	3438	46
H(26A)	550	9179	5986	202
H(26B)	1242	10069	5445	202
H(26C)	1468	9517	6483	202
H(27A)	4687	7951	4862	144
H(27B)	4196	8708	5741	144
H(27C)	3964	9260	4704	144
H(28A)	3384	6203	5841	138
H(28B)	1969	6591	6222	138
H(28C)	2872	6902	6754	138
H(32)	3920	4126	3879	57
H(33)	3047	3111	5176	74
H(34)	1108	2912	5201	89
H(35)	120	3648	3902	86
H(36)	969	4718	2610	63
H(42)	3040	3754	963	60
H(43)	2078	3812	-320	70
H(44)	822	5531	-888	70
H(45)	526	7203	-177	70
H(46)	1537	7175	1070	57

Table S5. Hydrogen coordinates ($x \ 10^4$) and isotropic displacement parameters (Å² x 10³) for **8**.



