
SUPPLEMENTARY MATERIAL

Table S1 - Crystal Data and Structure Refinement for **2**.

Table S2 - Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**.

Table S3 - Bond lengths (\AA) and angles (degrees) for **2**.

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Table S5 - Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**.

Table S6 - Weighted least-squares planes through the starred atoms for **2**.

Table S1' - Crystal Data and Structure Refinement for **3**.

Table S2' - Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3**.

Table S3' - Bond lengths (\AA) and angles (degrees) for **3**.

Table S4' - Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **3**.

Table S5' - Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3**.

Table S6' - Weighted least-squares planes through the starred atoms for **3**.

Table S1'' - Crystal Data and Structure Refinement for **4**.

Table S2'' - Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4**.

Table S3'' - Bond lengths (\AA) and angles (degrees) for **4**.

Table S4'' - Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **4**.

Table S5'' - Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4**.

Table S6'' - Weighted least-squares planes through the starred atoms for **4**.

Table S1''' - Crystal Data and Structure Refinement for **5**.

Table S2''' - Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**.

Table S3''' - Bond lengths (\AA) and angles (degrees) for **5**.

Table S4''' - Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **5**.

Table S5''' - Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**.

Table S6''' - Weighted least-squares planes through the starred atoms for **5**.

Figure S1 - ORTEP drawing of **2**.

Figure S2 - Unit cell and packing diagrams of **2**.

Figure S1' - ORTEP drawing of **3**.

Figure S2' - Unit cell and packing diagrams of **3**.

Figure S1'' - ORTEP drawing of **4**.

Figure S2'' - Unit cell and packing diagrams of **4**.

Figure S1''' - ORTEP drawing of **5**.

Figure S2''' - Unit cell and packing diagrams of **5**.

Table S1. Crystal data and structure refinement for 2.

Empirical formula	C ₁₄ H ₂₃ Cl ₂ S ₃ Ta
Formula weight	539.35
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P _b ca
Unit cell dimensions	a = 8.7870(10) Å alpha = 90 deg. b = 14.3020(10) Å beta = 90 deg. c = 28.5760(10) Å gamma = 90 deg.
Volume	3591.2(5) Å ³
Z, Calculated density	8, 1.995 Mg/m ³
Absorption coefficient	6.756 mm ⁻¹
F(000)	2096
Crystal size	0.2 x 0.2 x 0.1 mm
Theta range for data collection	2.72 to 27.97 deg.
Limiting indices	0 ≤ h ≤ 11, 0 ≤ k ≤ 18, 0 ≤ l ≤ 37
Reflections collected / unique	4324 / 4324 [R(int) = 0.0000]
Completeness to theta = 27.97	99.9 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4324 / 0 / 116
Goodness-of-fit on F ²	1.043
Final R indices [I > 2σ(I)]	R1 = 0.0759, wR2 = 0.2010
R indices (all data)	R1 = 0.1993, wR2 = 0.3016
Largest diff. peak and hole	3.716 and -3.442 e. Å ⁻³

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Ta(1)	4413(1)	1163(1)	8742(1)	23(1)
Cl(1)	6423(10)	1736(6)	9282(3)	55(2)
Cl(2)	6331(9)	1808(6)	8196(3)	52(2)
S(1)	3618(10)	227(6)	8077(3)	49(2)
S(2)	6634(8)	-80(5)	8709(3)	45(2)
S(3)	3629(9)	96(5)	9356(3)	39(2)
C(1)	5170(50)	-410(30)	7899(14)	67(11)
C(2)	5990(60)	-840(40)	8253(17)	93(15)
C(3)	6470(50)	-740(30)	9276(15)	78(12)
C(4)	4830(40)	-880(20)	9390(13)	52(8)
C(11)	2990(30)	2399(16)	9162(9)	20(6)
C(12)	3580(30)	2796(17)	8750(11)	34(5)
C(13)	2790(40)	2350(20)	8369(13)	46(9)
C(14)	1810(30)	1734(17)	8534(9)	26(5)
C(15)	1890(30)	1640(20)	9031(11)	40(7)
C(16)	3400(50)	2640(30)	9670(14)	69(12)
C(17)	4550(30)	3669(15)	8757(13)	31(5)
C(18)	2970(30)	2680(20)	7864(10)	38(7)
C(19)	580(30)	1251(18)	8248(9)	35(6)
C(20)	640(50)	1280(30)	9295(14)	65(10)

Table S3. Bond lengths [Å] and angles [°] for **2**.

Ta(1)-S(3)	2.425(7)
Ta(1)-S(1)	2.427(8)
Ta(1)-C(12)	2.45(2)
Ta(1)-C(13)	2.46(4)
Ta(1)-C(15)	2.46(3)
Ta(1)-C(11)	2.48(2)
Ta(1)-Cl(2)	2.475(7)
Ta(1)-Cl(1)	2.483(8)
Ta(1)-C(14)	2.50(2)
Ta(1)-S(2)	2.641(7)
S(1)-C(1)	1.72(4)
S(2)-C(2)	1.79(5)
S(2)-C(3)	1.88(4)
S(3)-C(4)	1.76(3)
C(1)-C(2)	1.38(6)
C(3)-C(4)	1.49(5)
C(11)-C(12)	1.41(4)
C(11)-C(15)	1.50(4)
C(11)-C(16)	1.53(5)
C(12)-C(13)	1.44(4)
C(12)-C(17)	1.51(3)
C(13)-C(14)	1.32(4)
C(13)-C(18)	1.53(4)
C(14)-C(15)	1.43(3)
C(14)-C(19)	1.53(4)
C(15)-C(20)	1.42(5)
S(3)-Ta(1)-S(1)	97.9(3)
S(3)-Ta(1)-C(12)	120.6(7)
S(1)-Ta(1)-C(12)	116.5(7)
S(3)-Ta(1)-C(13)	125.8(9)
S(1)-Ta(1)-C(13)	82.9(9)
C(12)-Ta(1)-C(13)	34.0(10)
S(3)-Ta(1)-C(15)	71.0(7)
S(1)-Ta(1)-C(15)	98.9(7)
C(12)-Ta(1)-C(15)	57.7(9)
C(13)-Ta(1)-C(15)	55.5(12)
S(3)-Ta(1)-C(11)	87.4(6)
S(1)-Ta(1)-C(11)	128.8(6)
C(12)-Ta(1)-C(11)	33.2(9)
C(13)-Ta(1)-C(11)	54.8(9)
C(15)-Ta(1)-C(11)	35.5(9)
S(3)-Ta(1)-Cl(2)	152.1(3)
S(1)-Ta(1)-Cl(2)	84.7(3)
C(12)-Ta(1)-Cl(2)	81.5(7)
C(13)-Ta(1)-Cl(2)	82.1(9)
C(15)-Ta(1)-Cl(2)	136.2(7)
C(11)-Ta(1)-Cl(2)	112.5(6)
S(3)-Ta(1)-Cl(1)	87.7(3)
S(1)-Ta(1)-Cl(1)	150.8(3)

C(12)-Ta(1)-Cl(1)	83.8(7)
C(13)-Ta(1)-Cl(1)	116.8(9)
C(15)-Ta(1)-Cl(1)	110.0(7)
C(11)-Ta(1)-Cl(1)	79.8(6)
Cl(2)-Ta(1)-Cl(1)	77.5(3)
S(3)-Ta(1)-C(14)	96.8(6)
S(1)-Ta(1)-C(14)	74.4(6)
C(12)-Ta(1)-C(14)	54.3(8)
C(13)-Ta(1)-C(14)	30.9(10)
C(15)-Ta(1)-C(14)	33.5(8)
C(11)-Ta(1)-C(14)	54.5(8)
Cl(2)-Ta(1)-C(14)	110.5(6)
Cl(1)-Ta(1)-C(14)	133.7(6)
S(3)-Ta(1)-S(2)	79.2(3)
S(1)-Ta(1)-S(2)	79.3(3)
C(12)-Ta(1)-S(2)	149.7(6)
C(13)-Ta(1)-S(2)	151.3(9)
C(15)-Ta(1)-S(2)	149.7(7)
C(11)-Ta(1)-S(2)	150.6(7)
Cl(2)-Ta(1)-S(2)	74.1(3)
Cl(1)-Ta(1)-S(2)	73.7(3)
C(14)-Ta(1)-S(2)	152.5(6)
C(1)-S(1)-Ta(1)	107.3(14)
C(2)-S(2)-C(3)	107(2)
C(2)-S(2)-Ta(1)	101.5(17)
C(3)-S(2)-Ta(1)	104.5(14)
C(4)-S(3)-Ta(1)	111.8(12)
C(2)-C(1)-S(1)	116(3)
C(1)-C(2)-S(2)	116(4)
C(4)-C(3)-S(2)	109(3)
C(3)-C(4)-S(3)	117(3)
C(12)-C(11)-C(15)	109(2)
C(12)-C(11)-C(16)	128(3)
C(15)-C(11)-C(16)	123(3)
C(12)-C(11)-Ta(1)	72.3(14)
C(15)-C(11)-Ta(1)	71.8(15)
C(16)-C(11)-Ta(1)	120(2)
C(11)-C(12)-C(13)	106(2)
C(11)-C(12)-C(17)	122(3)
C(13)-C(12)-C(17)	130(3)
C(11)-C(12)-Ta(1)	74.5(14)
C(13)-C(12)-Ta(1)	73.6(17)
C(17)-C(12)-Ta(1)	128.4(16)
C(14)-C(13)-C(12)	110(3)
C(14)-C(13)-C(18)	128(3)
C(12)-C(13)-C(18)	122(3)
C(14)-C(13)-Ta(1)	76.0(19)
C(12)-C(13)-Ta(1)	72.4(18)
C(18)-C(13)-Ta(1)	124(2)
C(13)-C(14)-C(15)	113(3)
C(13)-C(14)-C(19)	125(3)
C(15)-C(14)-C(19)	121(3)

C(13)-C(14)-Ta(1)	73.1(19)
C(15)-C(14)-Ta(1)	72.0(17)
C(19)-C(14)-Ta(1)	129.1(17)
C(20)-C(15)-C(14)	122(3)
C(20)-C(15)-C(11)	129(3)
C(14)-C(15)-C(11)	102(2)
C(20)-C(15)-Ta(1)	140(2)
C(14)-C(15)-Ta(1)	74.6(17)
<u>C(11)-C(15)-Ta(1)</u>	<u>72.7(15)</u>

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**. 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
Ta(1)	22(1)	24(1)	24(1)	0(1)	1(1)	1(1)
Cl(1)	45(4)	55(5)	64(6)	-11(4)	-18(4)	0(4)
Cl(2)	36(4)	55(5)	65(5)	11(4)	26(4)	0(4)
S(1)	45(4)	46(4)	55(5)	-25(4)	-9(4)	11(4)
S(2)	34(3)	43(4)	57(5)	5(4)	7(4)	13(3)
S(3)	37(4)	39(4)	39(4)	16(3)	8(3)	7(3)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**.

	x	y	z	U(eq)
H(1A)	4821	-890	7684	81
H(1B)	5845	0	7728	81
H(2A)	6867	-1140	8115	112
H(2B)	5359	-1321	8391	112
H(3A)	6971	-1344	9248	94
H(3B)	6959	-395	9525	94
H(4A)	4769	-1132	9706	63
H(4B)	4434	-1359	9181	63
H(16A)	4487	2672	9700	83
H(16B)	3017	2157	9873	83
H(16C)	2957	3226	9754	83
H(17A)	4194	4079	9000	37
H(17B)	4472	3980	8460	37
H(17C)	5588	3503	8815	37
H(18A)	2439	2262	7660	45
H(18B)	4027	2697	7783	45
H(18C)	2547	3300	7833	45
H(19A)	-405	1442	8360	42
H(19B)	677	585	8280	42
H(19C)	680	1420	7925	42
H(20A)	168	1773	9466	78
H(20B)	1012	812	9510	78
H(20C)	-83	996	9087	78

Table S6. Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane) for 2.

Plane 1

$$- 6.3619 (0.0763) x + 9.8363 (0.1330) y + 1.5092 (0.5163) z = 1.8096 (0.4506)$$

* 0.0326 (0.0166) C11

* -0.0169 (0.0160) C12

* -0.0089 (0.0188) C13

* 0.0298 (0.0208) C14

* -0.0366 (0.0183) C15

Rms deviation of fitted atoms = 0.0270

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

Empirical formula	C ₁₆ H ₂₉ O S ₂ Ta
Formula weight	482.46
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 8.6809(10) Å b = 14.970(3) Å c = 27.043(2) Å
Volume	3514.3(9) Å ³
Z	8
Density (calculated)	1.824 Mg/m ³
Absorption coefficient	6.487 mm ⁻¹
Transmission range	0.690-1.000
F(000)	1904
Crystal size	0.4 x 0.3 x 0.1 mm
Theta range for data collection	2.72 to 28.03°
Index ranges	0 ≤ h ≤ 11, 0 ≤ k ≤ 19, 0 ≤ l ≤ 35
Reflections collected	4244
Independent reflections	4244 [R(int) = 0.0000]
Completeness to theta = 28.03°	99.6 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4244 / 0 / 181
Goodness-of-fit on F ²	1.021
Final R indices [I > 2σ(I)]	R1 = 0.0512, wR2 = 0.0972
R indices (all data)	R1 = 0.1409, wR2 = 0.1163
Largest diff. peak and hole	1.076 and -1.050 e.Å ⁻³

Table S2'. 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(eq)
Ta(1)	1791(1)	1759(1)	3790(1)	32(1)
S(1)	852(3)	810(2)	4466(1)	43(1)
S(2)	1696(4)	3220(2)	4203(1)	49(1)
O(1)	3787(8)	1732(5)	4390(2)	40(2)
C(1)	2407(16)	705(9)	4902(4)	62(3)
C(2)	3877(16)	936(9)	4698(5)	71(4)
C(3)	4170(17)	2502(8)	4666(5)	66(4)
C(4)	3636(17)	3314(8)	4437(6)	77(5)
C(5)	3279(13)	618(7)	3546(4)	49(3)
C(6)	3756(13)	2367(9)	3376(5)	58(3)
C(11)	392(13)	2426(8)	3094(4)	48(3)
C(12)	-639(13)	2397(8)	3489(4)	44(3)
C(13)	-950(12)	1503(8)	3595(4)	42(3)
C(14)	-75(12)	975(7)	3268(4)	39(3)
C(15)	699(13)	1549(8)	2958(4)	49(3)
C(16)	889(18)	3237(10)	2816(6)	96(6)
C(17)	-1496(18)	3205(11)	3705(6)	104(6)
C(18)	-2182(13)	1183(13)	3947(5)	88(5)
C(19)	-199(17)	-18(8)	3241(6)	90(5)
C(20)	1580(16)	1228(11)	2495(5)	80(4)

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

Ta(1)-S(1)	2.455(3)
Ta(1)-S(2)	2.458(3)
Ta(1)-O(1)	2.375(6)
Ta(1)-C(5)	2.241(11)
Ta(1)-C(6)	2.233(12)
Ta(1)-C(11)	2.452(11)
Ta(1)-C(12)	2.455(10)
Ta(1)-C(13)	2.467(10)
Ta(1)-C(14)	2.447(10)
Ta(1)-C(15)	2.461(11)
S(1)-C(1)	1.799(12)
S(2)-C(4)	1.805(14)
O(1)-C(2)	1.455(14)
O(1)-C(3)	1.412(13)
C(1)-C(2)	1.433(17)
C(3)-C(4)	1.441(17)
C(11)-C(12)	1.394(15)
C(11)-C(15)	1.388(15)
C(11)-C(16)	1.493(16)
C(12)-C(13)	1.395(15)
C(12)-C(17)	1.535(16)
C(13)-C(14)	1.407(14)
C(13)-C(18)	1.511(16)
C(14)-C(15)	1.376(15)
C(14)-C(19)	1.492(15)
C(15)-C(20)	1.543(16)
C(6)-Ta(1)-C(5)	73.9(5)
C(6)-Ta(1)-O(1)	78.0(4)
C(5)-Ta(1)-O(1)	76.6(3)
C(6)-Ta(1)-C(14)	114.4(4)
C(5)-Ta(1)-C(14)	81.1(4)
O(1)-Ta(1)-C(14)	150.3(3)
C(6)-Ta(1)-C(11)	80.1(4)
C(5)-Ta(1)-C(11)	111.7(4)
O(1)-Ta(1)-C(11)	153.2(3)
C(14)-Ta(1)-C(11)	54.9(3)
C(6)-Ta(1)-C(12)	109.4(4)
C(5)-Ta(1)-C(12)	134.0(4)
O(1)-Ta(1)-C(12)	149.3(3)
C(14)-Ta(1)-C(12)	55.0(3)
C(11)-Ta(1)-C(12)	33.0(4)
C(6)-Ta(1)-S(1)	149.6(3)
C(5)-Ta(1)-S(1)	88.3(3)
O(1)-Ta(1)-S(1)	73.92(18)
C(14)-Ta(1)-S(1)	86.1(3)
C(11)-Ta(1)-S(1)	130.0(3)
C(12)-Ta(1)-S(1)	100.8(3)
C(6)-Ta(1)-S(2)	83.7(4)
C(5)-Ta(1)-S(2)	146.3(3)
O(1)-Ta(1)-S(2)	74.27(19)
C(14)-Ta(1)-S(2)	131.8(2)
C(11)-Ta(1)-S(2)	88.3(3)
C(12)-Ta(1)-S(2)	77.0(3)
S(1)-Ta(1)-S(2)	99.50(10)

C(6)-Ta(1)-C(15)	83.6(4)
C(5)-Ta(1)-C(15)	81.7(4)
O(1)-Ta(1)-C(15)	154.7(3)
C(14)-Ta(1)-C(15)	32.6(3)
C(11)-Ta(1)-C(15)	32.8(4)
C(12)-Ta(1)-C(15)	54.2(4)
S(1)-Ta(1)-C(15)	118.6(3)
S(2)-Ta(1)-C(15)	121.1(3)
C(6)-Ta(1)-C(13)	133.9(4)
C(5)-Ta(1)-C(13)	112.0(4)
O(1)-Ta(1)-C(13)	147.9(3)
C(14)-Ta(1)-C(13)	33.3(3)
C(11)-Ta(1)-C(13)	54.6(4)
C(12)-Ta(1)-C(13)	32.9(4)
S(1)-Ta(1)-C(13)	75.5(3)
S(2)-Ta(1)-C(13)	101.7(3)
C(15)-Ta(1)-C(13)	54.1(4)
C(1)-S(1)-Ta(1)	106.9(4)
C(4)-S(2)-Ta(1)	101.4(5)
C(3)-O(1)-C(2)	110.7(9)
C(3)-O(1)-Ta(1)	121.3(7)
C(2)-O(1)-Ta(1)	116.3(7)
C(2)-C(1)-S(1)	113.2(9)
C(1)-C(2)-O(1)	111.8(10)
O(1)-C(3)-C(4)	112.7(11)
C(3)-C(4)-S(2)	112.7(9)
C(15)-C(11)-C(12)	107.3(10)
C(15)-C(11)-C(16)	125.5(13)
C(12)-C(11)-C(16)	126.6(13)
C(15)-C(11)-Ta(1)	74.0(7)
C(12)-C(11)-Ta(1)	73.6(6)
C(16)-C(11)-Ta(1)	125.1(8)
C(11)-C(12)-C(13)	108.1(10)
C(11)-C(12)-C(17)	125.4(12)
C(13)-C(12)-C(17)	125.7(12)
C(11)-C(12)-Ta(1)	73.4(6)
C(13)-C(12)-Ta(1)	74.0(6)
C(17)-C(12)-Ta(1)	126.6(8)
C(12)-C(13)-C(14)	107.8(10)
C(12)-C(13)-C(18)	124.8(12)
C(14)-C(13)-C(18)	126.8(12)
C(12)-C(13)-Ta(1)	73.1(6)
C(14)-C(13)-Ta(1)	72.6(6)
C(18)-C(13)-Ta(1)	126.7(7)
C(15)-C(14)-C(13)	107.2(9)
C(15)-C(14)-C(19)	128.8(13)
C(13)-C(14)-C(19)	123.5(12)
C(15)-C(14)-Ta(1)	74.3(6)
C(13)-C(14)-Ta(1)	74.1(6)
C(19)-C(14)-Ta(1)	123.7(8)
C(14)-C(15)-C(11)	109.6(10)
C(14)-C(15)-C(20)	122.8(11)
C(11)-C(15)-C(20)	127.2(12)
C(14)-C(15)-Ta(1)	73.2(6)
C(11)-C(15)-Ta(1)	73.2(7)
C(20)-C(15)-Ta(1)	126.1(8)

Table S4'. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3. The anisotropic displacement factor exponent takes the form:**

$$-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	31(1)	32(1)	32(1)	1(1)	-1(1)	0(1)
S(1)	46(2)	44(2)	40(2)	8(1)	-4(1)	-5(1)
S(2)	67(2)	37(1)	45(1)	-5(2)	-4(2)	1(2)
O(1)	46(4)	42(4)	31(3)	-2(4)	-9(3)	-2(4)
C(1)	59(7)	65(8)	62(8)	27(7)	-24(7)	-16(6)
C(2)	61(8)	73(10)	81(11)	29(9)	-27(8)	8(8)
C(3)	76(10)	50(8)	71(10)	-10(7)	-16(8)	2(7)
C(4)	98(11)	33(6)	101(11)	3(8)	-41(9)	-20(7)
C(5)	42(6)	54(6)	51(6)	2(6)	-5(6)	11(6)
C(6)	39(6)	64(8)	70(9)	12(8)	-9(6)	-4(6)
C(11)	48(7)	53(7)	44(7)	10(6)	-22(6)	-18(6)
C(12)	43(7)	53(7)	35(6)	-12(6)	-2(5)	15(6)
C(13)	32(5)	65(8)	29(5)	12(5)	-5(4)	-2(5)
C(14)	44(6)	31(5)	43(7)	-7(5)	-15(5)	6(5)
C(15)	45(6)	59(8)	43(6)	-3(6)	-8(5)	5(6)
C(16)	101(11)	85(10)	100(12)	61(10)	-67(10)	-36(10)
C(17)	90(11)	118(13)	104(13)	-36(12)	-38(10)	68(11)
C(18)	33(7)	159(16)	71(10)	38(10)	-6(6)	-5(8)
C(19)	92(11)	43(7)	135(14)	-10(8)	-57(11)	-5(8)
C(20)	65(9)	119(11)	54(8)	-30(9)	-3(7)	27(9)

Table S5'. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 3.

	x	y	z	U(eq)
H(1A)	2201	1088	5184	74
H(1B)	2446	94	5020	74
H(2A)	4257	441	4501	86
H(2B)	4603	1039	4964	86
H(3A)	5280	2531	4704	79
H(3B)	3721	2453	4993	79
H(4A)	4322	3468	4167	93
H(4B)	3677	3794	4677	93
H(5A)	2827	65	3652	73
H(5B)	4286	679	3689	73
H(5C)	3362	621	3192	73
H(6A)	3644	3005	3372	87
H(6B)	3762	2146	3043	87
H(6C)	4707	2212	3536	87
H(16A)	557	3762	2989	143
H(16B)	439	3230	2492	143
H(16C)	1991	3242	2788	143
H(17A)	-1055	3746	3577	156
H(17B)	-1404	3200	4059	156
H(17C)	-2564	3175	3614	156
H(18A)	-2181	542	3956	132
H(18B)	-3170	1391	3837	132
H(18C)	-1977	1412	4272	132
H(19A)	495	-239	2993	135
H(19B)	-1235	-181	3156	135
H(19C)	64	-272	3556	135
H(20A)	1596	587	2489	119
H(20B)	2617	1450	2506	119
H(20C)	1076	1447	2204	119

Table S6'. Weighted least-squares planes through the starred atoms for 3.
(Nardelli Musatti Domiano & Andreotti Ric.Sci.(1965) 15(II-A) 807).
Equation of the plane: $m_1 \cdot X + m_2 \cdot Y + m_3 \cdot Z = d$

Plane 1

$$m_1 = -0.76783(0.00385)$$

$$m_2 = 0.00782(0.00540)$$

$$m_3 = -0.64061(0.00461)$$

$$D = -5.58629(0.04407)$$

Atom	d	s	d/s	(d/s)**2
C11*	-0.0065	0.0115	-0.566	0.320
C12*	-0.0034	0.0110	-0.307	0.094
C13*	0.0098	0.0103	0.953	0.908
C14*	-0.0144	0.0108	-1.336	1.784
C15*	0.0142	0.0114	1.239	1.535
Sum ((d/s)**2) for starred atoms				4.641
Chi-squared at 95% for 2 degrees of freedom:				5.99

Table S1''. Crystal data and structure refinement for 4.

Empirical formula	C ₃₂ H ₅₈ S ₆ Ta ₂
Formula weight	997.04
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 14.1220(10) Å alpha = 90 deg. b = 8.9040(10) Å beta = 102.45(1) deg. c = 30.4000(10) Å gamma = 90 deg.
Volume	3732.7(5) Å ³
Z, Calculated density	4, 1.774 Mg/m ³
Absorption coefficient	6.215 mm ⁻¹
F(000)	1968
Crystal size	0.2 x 0.2 x 0.1 mm
Theta range for data collection	2.26 to 28.01 deg.
Limiting indices	-18 ≤ h ≤ 18, 0 ≤ k ≤ 11, 0 ≤ l ≤ 40
Reflections collected / unique	9137 / 8984 [R(int) = 0.0304]
Completeness to theta = 28.01	99.6 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8984 / 0 / 361
Goodness-of-fit on F ²	1.060
Final R indices [I > 2sigma(I)]	R1 = 0.0681, wR2 = 0.1996
R indices (all data)	R1 = 0.1296, wR2 = 0.2795
Largest diff. peak and hole	6.057 and -5.544 e. Å ⁻³

Table S2''. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^j tensor.

	x	y	z	U(eq)
Ta(1)	3445(1)	8698(1)	1318(1)	33(1)
S(1)	1979(3)	9330(5)	743(2)	51(1)
S(2)	2241(3)	6544(5)	1425(2)	48(1)
S(3)	2862(3)	9538(5)	1987(2)	52(1)
C(1)	1146(14)	7810(20)	708(9)	74(7)
C(2)	1034(13)	7170(20)	1120(7)	62(5)
C(3)	2132(17)	6650(30)	2002(8)	75(7)
C(4)	2018(18)	8220(30)	2151(7)	75(7)
C(5)	3615(13)	6910(20)	804(6)	49(4)
C(6)	4346(13)	6950(20)	1750(8)	61(5)
C(11)	4316(16)	11050(20)	1572(7)	59(5)
C(12)	3793(12)	11311(17)	1117(7)	47(4)
C(13)	4177(11)	10384(17)	840(7)	47(4)
C(14)	4943(11)	9555(19)	1103(6)	45(4)
C(15)	5035(12)	9970(20)	1557(6)	52(4)
C(16)	4350(20)	11950(30)	1992(11)	115(13)
C(17)	3055(15)	12530(20)	981(14)	133(16)
C(18)	3921(17)	10420(30)	324(8)	82(7)
C(19)	5670(15)	8580(20)	936(10)	80(8)
C(20)	5852(17)	9520(40)	1928(10)	102(10)
Ta(1A)	8324(1)	13793(1)	1136(1)	37(1)
S(1A)	9663(3)	14371(6)	1778(2)	56(1)
S(2A)	9553(3)	11623(5)	1106(2)	60(1)
S(3A)	9110(3)	14657(5)	528(2)	51(1)
C(1A)	10436(16)	12710(30)	1906(7)	77(7)
C(2A)	10686(14)	12110(30)	1488(8)	69(6)
C(3A)	9910(15)	11820(20)	566(8)	67(6)
C(4A)	10109(15)	13450(20)	464(9)	67(6)
C(5A)	7993(16)	11970(20)	1601(9)	69(6)
C(6A)	7513(13)	12079(19)	646(8)	65(6)
C(11A)	7695(11)	16361(18)	939(7)	48(4)
C(12A)	7874(12)	16241(19)	1415(7)	51(4)
C(13A)	7215(14)	15140(20)	1519(7)	58(5)
C(14A)	6634(11)	14632(19)	1109(7)	52(5)
C(15A)	6950(11)	15371(18)	760(6)	47(4)
C(16A)	8099(18)	17580(20)	689(12)	102(11)
C(17A)	8504(16)	17250(30)	1794(10)	93(9)
C(18A)	7034(18)	14830(30)	1975(8)	88(8)
C(19A)	5758(15)	13640(20)	1061(12)	90(9)
C(20A)	6509(17)	15280(30)	281(9)	82(7)

Table S3''. Bond lengths [Å] and angles [°] for 4.

Ta(1)-C(6)	2.249(18)
Ta(1)-C(5)	2.280(17)
Ta(1)-C(11)	2.465(18)
Ta(1)-C(13)	2.467(15)
Ta(1)-C(14)	2.467(15)
Ta(1)-S(3)	2.468(4)
Ta(1)-S(1)	2.470(4)
Ta(1)-C(15)	2.478(17)
Ta(1)-C(12)	2.482(15)
Ta(1)-S(2)	2.629(4)
S(1)-C(1)	1.782(19)
S(2)-C(3)	1.79(2)
S(2)-C(2)	1.84(2)
S(3)-C(4)	1.814(19)
C(1)-C(2)	1.41(3)
C(3)-C(4)	1.49(3)
C(11)-C(15)	1.41(3)
C(11)-C(12)	1.44(3)
C(11)-C(16)	1.50(3)
C(12)-C(13)	1.37(2)
C(12)-C(17)	1.50(2)
C(13)-C(14)	1.41(2)
C(13)-C(18)	1.53(3)
C(14)-C(15)	1.41(3)
C(14)-C(19)	1.51(2)
C(15)-C(20)	1.48(3)
Ta(1A)-C(6A)	2.263(18)
Ta(1A)-C(5A)	2.27(2)
Ta(1A)-C(13A)	2.455(18)
Ta(1A)-S(1A)	2.462(5)
Ta(1A)-C(15A)	2.467(14)
Ta(1A)-C(12A)	2.472(16)
Ta(1A)-S(3A)	2.475(5)
Ta(1A)-C(11A)	2.478(15)
Ta(1A)-C(14A)	2.485(14)
Ta(1A)-S(2A)	2.612(4)
S(1A)-C(1A)	1.83(2)
S(2A)-C(2A)	1.82(2)
S(2A)-C(3A)	1.83(2)
S(3A)-C(4A)	1.819(19)
C(1A)-C(2A)	1.49(3)
C(3A)-C(4A)	1.52(3)
C(11A)-C(15A)	1.39(2)
C(11A)-C(12A)	1.42(3)
C(11A)-C(16A)	1.51(3)
C(12A)-C(13A)	1.43(3)
C(12A)-C(17A)	1.58(3)
C(13A)-C(14A)	1.41(3)
C(13A)-C(18A)	1.49(3)

C(14A)-C(15A)	1.40(3)
C(14A)-C(19A)	1.50(2)
C(15A)-C(20A)	1.45(3)
C(6)-Ta(1)-C(5)	77.6(8)
C(6)-Ta(1)-C(11)	103.0(8)
C(5)-Ta(1)-C(11)	133.5(6)
C(6)-Ta(1)-C(13)	120.7(6)
C(5)-Ta(1)-C(13)	84.4(6)
C(11)-Ta(1)-C(13)	54.8(6)
C(6)-Ta(1)-C(14)	87.7(6)
C(5)-Ta(1)-C(14)	79.1(6)
C(11)-Ta(1)-C(14)	54.7(6)
C(13)-Ta(1)-C(14)	33.1(5)
C(6)-Ta(1)-S(3)	88.7(6)
C(5)-Ta(1)-S(3)	151.5(5)
C(11)-Ta(1)-S(3)	73.6(4)
C(13)-Ta(1)-S(3)	123.9(4)
C(14)-Ta(1)-S(3)	125.6(4)
C(6)-Ta(1)-S(1)	148.6(5)
C(5)-Ta(1)-S(1)	82.5(5)
C(11)-Ta(1)-S(1)	108.3(6)
C(13)-Ta(1)-S(1)	80.6(4)
C(14)-Ta(1)-S(1)	112.1(4)
S(3)-Ta(1)-S(1)	97.88(17)
C(6)-Ta(1)-C(15)	77.4(6)
C(5)-Ta(1)-C(15)	107.2(6)
C(11)-Ta(1)-C(15)	33.1(6)
C(13)-Ta(1)-C(15)	55.0(6)
C(14)-Ta(1)-C(15)	33.1(6)
S(3)-Ta(1)-C(15)	93.6(5)
S(1)-Ta(1)-C(15)	132.2(4)
C(6)-Ta(1)-C(12)	132.6(6)
C(5)-Ta(1)-C(12)	115.5(6)
C(11)-Ta(1)-C(12)	33.8(7)
C(13)-Ta(1)-C(12)	32.2(5)
C(14)-Ta(1)-C(12)	54.4(5)
S(3)-Ta(1)-C(12)	92.2(4)
S(1)-Ta(1)-C(12)	78.0(5)
C(15)-Ta(1)-C(12)	55.2(6)
C(6)-Ta(1)-S(2)	73.8(5)
C(5)-Ta(1)-S(2)	75.0(5)
C(11)-Ta(1)-S(2)	150.8(4)
C(13)-Ta(1)-S(2)	151.8(4)
C(14)-Ta(1)-S(2)	150.8(4)
S(3)-Ta(1)-S(2)	77.28(14)
S(1)-Ta(1)-S(2)	77.75(15)
C(15)-Ta(1)-S(2)	150.0(4)
C(12)-Ta(1)-S(2)	151.9(4)
C(1)-S(1)-Ta(1)	108.1(8)
C(3)-S(2)-C(2)	102.2(11)
C(3)-S(2)-Ta(1)	106.0(6)
C(2)-S(2)-Ta(1)	105.6(6)

C(4)-S(3)-Ta(1)	112.7(7)
C(2)-C(1)-S(1)	116.8(17)
C(1)-C(2)-S(2)	107.4(14)
C(4)-C(3)-S(2)	112.6(15)
C(3)-C(4)-S(3)	113.7(15)
C(15)-C(11)-C(12)	107.7(16)
C(15)-C(11)-C(16)	120(2)
C(12)-C(11)-C(16)	130(2)
C(15)-C(11)-Ta(1)	74.0(10)
C(12)-C(11)-Ta(1)	73.7(10)
C(16)-C(11)-Ta(1)	129.9(13)
C(13)-C(12)-C(11)	107.6(15)
C(13)-C(12)-C(17)	128(2)
C(11)-C(12)-C(17)	124(2)
C(13)-C(12)-Ta(1)	73.3(9)
C(11)-C(12)-Ta(1)	72.4(9)
C(17)-C(12)-Ta(1)	125.6(12)
C(12)-C(13)-C(14)	109.0(17)
C(12)-C(13)-C(18)	125.4(18)
C(14)-C(13)-C(18)	125.0(18)
C(12)-C(13)-Ta(1)	74.5(9)
C(14)-C(13)-Ta(1)	73.4(9)
C(18)-C(13)-Ta(1)	125.4(12)
C(15)-C(14)-C(13)	108.5(15)
C(15)-C(14)-C(19)	123.5(19)
C(13)-C(14)-C(19)	127.2(19)
C(15)-C(14)-Ta(1)	73.9(9)
C(13)-C(14)-Ta(1)	73.4(8)
C(19)-C(14)-Ta(1)	126.5(13)
C(14)-C(15)-C(11)	107.2(17)
C(14)-C(15)-C(20)	125(2)
C(11)-C(15)-C(20)	127(2)
C(14)-C(15)-Ta(1)	73.0(10)
C(11)-C(15)-Ta(1)	72.9(10)
C(20)-C(15)-Ta(1)	127.5(13)
C(6A)-Ta(1A)-C(5A)	77.5(9)
C(6A)-Ta(1A)-C(13A)	110.9(7)
C(5A)-Ta(1A)-C(13A)	79.4(7)
C(6A)-Ta(1A)-S(1A)	148.9(5)
C(5A)-Ta(1A)-S(1A)	83.2(6)
C(13A)-Ta(1A)-S(1A)	88.9(6)
C(6A)-Ta(1A)-C(15A)	81.0(7)
C(5A)-Ta(1A)-C(15A)	116.8(7)
C(13A)-Ta(1A)-C(15A)	54.9(6)
S(1A)-Ta(1A)-C(15A)	129.9(4)
C(6A)-Ta(1A)-C(12A)	133.6(6)
C(5A)-Ta(1A)-C(12A)	108.4(8)
C(13A)-Ta(1A)-C(12A)	33.9(6)
S(1A)-Ta(1A)-C(12A)	75.7(4)
C(15A)-Ta(1A)-C(12A)	54.7(6)
C(6A)-Ta(1A)-S(3A)	87.9(6)
C(5A)-Ta(1A)-S(3A)	150.9(6)

C(13A)-Ta(1A)-S(3A)	129.6(4)
S(1A)-Ta(1A)-S(3A)	97.80(17)
C(15A)-Ta(1A)-S(3A)	84.9(4)
C(12A)-Ta(1A)-S(3A)	99.9(5)
C(6A)-Ta(1A)-C(11A)	111.1(7)
C(5A)-Ta(1A)-C(11A)	134.5(7)
C(13A)-Ta(1A)-C(11A)	55.5(6)
S(1A)-Ta(1A)-C(11A)	99.9(5)
C(15A)-Ta(1A)-C(11A)	32.7(6)
C(12A)-Ta(1A)-C(11A)	33.3(7)
S(3A)-Ta(1A)-C(11A)	74.2(4)
C(6A)-Ta(1A)-C(14A)	80.5(7)
C(5A)-Ta(1A)-C(14A)	84.9(7)
C(13A)-Ta(1A)-C(14A)	33.1(7)
S(1A)-Ta(1A)-C(14A)	122.1(5)
C(15A)-Ta(1A)-C(14A)	32.9(6)
C(12A)-Ta(1A)-C(14A)	55.2(6)
S(3A)-Ta(1A)-C(14A)	117.7(5)
C(11A)-Ta(1A)-C(14A)	54.8(5)
C(6A)-Ta(1A)-S(2A)	74.0(5)
C(5A)-Ta(1A)-S(2A)	73.6(6)
C(13A)-Ta(1A)-S(2A)	150.8(4)
S(1A)-Ta(1A)-S(2A)	77.23(17)
C(15A)-Ta(1A)-S(2A)	150.2(5)
C(12A)-Ta(1A)-S(2A)	152.4(4)
S(3A)-Ta(1A)-S(2A)	78.23(16)
C(11A)-Ta(1A)-S(2A)	151.7(4)
C(14A)-Ta(1A)-S(2A)	149.6(4)
C(1A)-S(1A)-Ta(1A)	108.8(8)
C(2A)-S(2A)-C(3A)	100.2(11)
C(2A)-S(2A)-Ta(1A)	107.5(7)
C(3A)-S(2A)-Ta(1A)	105.9(6)
C(4A)-S(3A)-Ta(1A)	112.2(7)
C(2A)-C(1A)-S(1A)	110.4(15)
C(1A)-C(2A)-S(2A)	107.1(14)
C(4A)-C(3A)-S(2A)	111.9(15)
C(3A)-C(4A)-S(3A)	111.2(13)
C(15A)-C(11A)-C(12A)	107.9(15)
C(15A)-C(11A)-C(16A)	126(2)
C(12A)-C(11A)-C(16A)	124(2)
C(15A)-C(11A)-Ta(1A)	73.2(9)
C(12A)-C(11A)-Ta(1A)	73.1(9)
C(16A)-C(11A)-Ta(1A)	129.2(11)
C(11A)-C(12A)-C(13A)	107.1(16)
C(11A)-C(12A)-C(17A)	131(2)
C(13A)-C(12A)-C(17A)	121(2)
C(11A)-C(12A)-Ta(1A)	73.6(9)
C(13A)-C(12A)-Ta(1A)	72.4(10)
C(17A)-C(12A)-Ta(1A)	127.5(12)
C(14A)-C(13A)-C(12A)	107.8(17)
C(14A)-C(13A)-C(18A)	125(2)
C(12A)-C(13A)-C(18A)	125(2)

C(14A)-C(13A)-Ta(1A)	74.6(10)
C(12A)-C(13A)-Ta(1A)	73.8(10)
C(18A)-C(13A)-Ta(1A)	127.5(13)
C(15A)-C(14A)-C(13A)	107.5(16)
C(15A)-C(14A)-C(19A)	126(2)
C(13A)-C(14A)-C(19A)	126(2)
C(15A)-C(14A)-Ta(1A)	72.9(8)
C(13A)-C(14A)-Ta(1A)	72.3(9)
C(19A)-C(14A)-Ta(1A)	126.2(12)
C(11A)-C(15A)-C(14A)	109.7(17)
C(11A)-C(15A)-C(20A)	123.5(19)
C(14A)-C(15A)-C(20A)	126.4(19)
C(11A)-C(15A)-Ta(1A)	74.1(9)
C(14A)-C(15A)-Ta(1A)	74.2(9)
C(20A)-C(15A)-Ta(1A)	123.8(12)

Table S4''. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4. 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
Ta(1)	35(1)	32(1)	34(1)	0(1)	11(1)	2(1)
S(1)	41(2)	50(2)	58(3)	7(2)	2(2)	1(2)
S(2)	58(2)	42(2)	42(3)	3(2)	9(2)	-10(2)
S(3)	49(2)	60(2)	53(3)	-9(2)	26(2)	-10(2)
C(1)	47(10)	68(12)	100(20)	-4(13)	-1(11)	-17(9)
C(2)	51(10)	72(12)	59(14)	-3(11)	3(9)	-25(9)
C(3)	81(14)	91(15)	52(14)	6(12)	11(11)	-47(12)
C(4)	105(17)	92(15)	35(11)	-1(11)	32(12)	-38(14)
C(5)	56(9)	51(9)	39(10)	-1(8)	8(8)	3(7)
C(6)	46(9)	52(10)	82(17)	12(10)	8(9)	5(7)
C(11)	81(13)	48(9)	62(13)	-12(9)	45(11)	-16(9)
C(12)	44(8)	42(8)	60(12)	8(8)	25(8)	0(6)
C(13)	41(7)	38(7)	61(13)	11(8)	11(8)	-10(6)
C(14)	42(7)	52(8)	47(11)	5(8)	22(7)	6(6)
C(15)	46(8)	67(11)	43(11)	18(9)	11(8)	-14(8)
C(16)	140(20)	86(17)	140(30)	-62(19)	90(20)	-74(18)
C(17)	50(11)	32(9)	320(50)	13(17)	48(19)	14(8)
C(18)	72(13)	95(17)	80(19)	24(14)	22(13)	-16(12)
C(19)	59(11)	67(12)	120(20)	-8(13)	46(14)	16(9)
C(20)	73(15)	130(20)	90(20)	17(19)	-1(14)	-49(16)
Ta(1A)	31(1)	33(1)	47(1)	2(1)	7(1)	1(1)
S(1A)	40(2)	66(3)	55(3)	-4(2)	-2(2)	6(2)
S(2A)	52(2)	44(2)	85(4)	3(2)	16(2)	16(2)
S(3A)	49(2)	51(2)	58(3)	6(2)	19(2)	8(2)
C(1A)	66(12)	120(20)	37(12)	5(13)	-5(9)	28(13)
C(2A)	54(10)	85(14)	66(15)	19(12)	6(10)	30(10)
C(3A)	66(11)	71(12)	71(16)	-1(11)	29(11)	24(10)
C(4A)	65(12)	69(12)	79(16)	-1(11)	41(12)	7(9)
C(5A)	75(13)	54(11)	84(18)	7(11)	32(12)	-5(9)
C(6A)	52(10)	41(8)	97(18)	-14(10)	8(10)	-5(7)
C(11A)	40(8)	46(8)	62(12)	7(8)	17(8)	9(6)
C(12A)	41(8)	53(9)	51(11)	-17(9)	-11(7)	7(7)
C(13A)	63(10)	57(10)	57(13)	25(10)	19(10)	25(9)
C(14A)	37(7)	49(8)	75(14)	12(9)	20(8)	10(6)
C(15A)	42(7)	47(8)	46(11)	6(8)	1(7)	19(7)
C(16A)	87(15)	34(9)	210(40)	14(14)	80(20)	11(9)
C(17A)	69(13)	63(13)	130(30)	-43(15)	-20(14)	2(10)
C(18A)	83(15)	110(20)	65(17)	2(15)	13(13)	42(15)
C(19A)	50(10)	50(10)	180(30)	11(14)	43(15)	-1(8)
C(20A)	77(14)	74(14)	100(20)	19(13)	15(13)	43(11)

Table S5'. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4.

	x	y	z	U(eq)
H(1A)	516	8155	547	89
H(1B)	1350	7020	529	89
H(2A)	592	6326	1062	74
H(2B)	771	7908	1296	74
H(3A)	1576	6065	2038	90
H(3B)	2705	6214	2192	90
H(4A)	2107	8239	2476	90
H(4B)	1362	8557	2024	90
H(5A)	4268	6537	872	59
H(5B)	3474	7339	508	59
H(5C)	3174	6096	817	59
H(6A)	3937	6131	1800	73
H(6B)	4655	7380	2034	73
H(6C)	4832	6577	1600	73
H(16A)	4386	11286	2243	138
H(16B)	3773	12552	1956	138
H(16C)	4908	12593	2044	138
H(17A)	3351	13372	868	160
H(17B)	2809	12833	1238	160
H(17C)	2532	12157	751	160
H(18A)	3229	10399	221	98
H(18B)	4198	9558	208	98
H(18C)	4175	11318	219	98
H(19A)	6226	9174	914	95
H(19B)	5378	8185	644	95
H(19C)	5867	7767	1142	95
H(20A)	6223	8748	1824	122
H(20B)	5604	9160	2178	122
H(20C)	6260	10380	2021	122
H(1C)	11026	12978	2121	92
H(1D)	10102	11948	2042	92
H(2C)	11098	11234	1556	83
H(2D)	11028	12867	1353	83
H(3C)	10488	11229	570	80
H(3D)	9397	11432	328	80
H(4C)	10204	13523	158	80
H(4D)	10700	13778	667	80
H(5D)	7318	11710	1519	83
H(5E)	8146	12322	1906	83
H(5F)	8377	11092	1576	83
H(6D)	7799	11107	716	78
H(6E)	7549	12352	344	78
H(6F)	6846	12053	670	78
H(16D)	7879	17412	365	123
H(16E)	8791	17561	761	123
H(16F)	7868	18542	759	123
H(17D)	9163	17257	1759	111
H(17E)	8478	16859	2085	111

H(17F)	8255	18261	1768	111
H(18D)	6711	15675	2073	105
H(18E)	7640	14660	2183	105
H(18F)	6632	13954	1962	105
H(19D)	5948	12676	1194	109
H(19E)	5467	13510	748	109
H(19F)	5297	14092	1211	109
H(20D)	5981	15981	210	99
H(20E)	6271	14282	209	99
H(20F)	6984	15522	109	99

Table S6''. Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane) for 4.

Plane 1.

$$9.6563 (0.0841) x + 6.4252 (0.0510) y - 7.6959 (0.2380) z = 10.0638 (0.0443)$$

- * -0.0069 (0.0099) C11
- * 0.0073 (0.0096) C12
- * -0.0048 (0.0095) C13
- * 0.0004 (0.0097) C14
- * 0.0041 (0.0101) C15

Rms deviation of fitted atoms = 0.0053

Plane 2.

$$- 9.7342 (0.0808) x + 6.4458 (0.0485) y + 5.3592 (0.2399) z = 3.5571 (0.1326)$$

- * 0.0012 (0.0096) C11A
- * 0.0055 (0.0098) C12A
- * -0.0102 (0.0100) C13A
- * 0.0110 (0.0097) C14A
- * -0.0077 (0.0094) C15A

Rms deviation of fitted atoms = 0.0080

Table S1''''. Crystal data and structure refinement for 5.

Empirical formula	C ₃₄ H ₄₇ N ₂ O ₂ Ta
Formula weight	744.81
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 8.723(2) Å alpha = 81.63(3) deg. b = 13.193(3) Å beta = 83.40(3) deg. c = 14.402(3) Å gamma = 80.56(3) deg.
Volume	1610.5(6) Å ³
Z, Calculated density	2, 1.536 Mg/m ³
Absorption coefficient	3.571 mm ⁻¹
F(000)	756
Crystal size	0.2 x 0.3 x 0.3 mm
Theta range for data collection	2.27 to 28.10 deg.
Limiting indices	-11 ≤ h ≤ 11, -17 ≤ k ≤ 17, 0 ≤ l ≤ 19
Reflections collected / unique	8108 / 7800 [R(int) = 0.0679]
Completeness to theta = 28.10	99.2 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7800 / 0 / 372
Goodness-of-fit on F ²	1.460
Final R indices [I > 2σ(I)]	R1 = 0.0678, wR2 = 0.1418
R indices (all data)	R1 = 0.1351, wR2 = 0.1717
Largest diff. peak and hole	3.945 and -2.633 e. Å ⁻³

Table S2''''. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ta(1)	6934(1)	7232(1)	7746(1)	28(1)
S(1)	9107(3)	6450(2)	8724(2)	41(1)
S(2)	4191(3)	7163(2)	7523(2)	41(1)
O(1)	5741(8)	6772(6)	9242(5)	37(2)
N(1)	7863(10)	6742(7)	6517(6)	35(2)
N(2)	6559(11)	4749(6)	8211(6)	35(2)
C(1)	8125(13)	5737(9)	9713(8)	39(2)
C(2)	6588(15)	6334(10)	10037(8)	53(3)
C(3)	4088(13)	6703(10)	9416(8)	48(3)
C(4)	3539(14)	6419(9)	8582(9)	48(3)
C(5)	7026(12)	5541(8)	7652(7)	33(2)
C(6)	7768(14)	5584(8)	6702(7)	35(2)
C(7)	9418(15)	4932(8)	6642(9)	48(3)
C(8)	6889(16)	5235(9)	5965(8)	48(3)
C(11)	7520(18)	9008(8)	6871(9)	54(4)
C(12)	8367(15)	8788(8)	7705(11)	54(4)
C(13)	7151(17)	8815(8)	8486(9)	48(3)
C(14)	5768(17)	9014(9)	8098(10)	54(4)
C(15)	5962(15)	9111(8)	7145(9)	44(3)
C(16)	8290(30)	9406(11)	5917(11)	108(8)
C(17)	10046(18)	8774(12)	7788(17)	115(8)
C(18)	7520(30)	8840(13)	9483(13)	127(9)
C(19)	4150(20)	9281(12)	8671(16)	120(9)
C(20)	4700(20)	9509(12)	6511(15)	112(8)
C(21)	8504(13)	7119(8)	5589(7)	36(2)
C(22)	10095(14)	7187(9)	5414(8)	42(3)
C(23)	10674(15)	7544(9)	4491(9)	52(3)
C(24)	9738(18)	7903(11)	3805(9)	60(4)
C(25)	8163(18)	7879(10)	3991(8)	56(4)
C(26)	7479(14)	7487(8)	4877(8)	39(3)
C(27)	11271(15)	6853(11)	6110(9)	57(3)
C(28)	5765(15)	7515(10)	5014(9)	56(3)
C(31)	6652(13)	3724(8)	8033(8)	38(3)
C(32)	7890(14)	2984(9)	8359(8)	44(3)
C(33)	7877(18)	1964(9)	8349(10)	60(4)
C(34)	6650(20)	1618(10)	7996(11)	73(5)
C(35)	5432(18)	2351(11)	7656(10)	64(4)
C(36)	5429(15)	3390(9)	7688(8)	44(3)
C(37)	9255(14)	3290(10)	8754(9)	51(3)
C(38)	4015(15)	4120(10)	7369(9)	55(3)

Table S3'' Bond lengths [Å] and angles [°] for 5.

Ta(1)-N(1)	2.010(9)
Ta(1)-C(5)	2.244(10)
Ta(1)-O(1)	2.324(7)
Ta(1)-S(2)	2.468(3)
Ta(1)-S(1)	2.488(3)
Ta(1)-C(14)	2.502(11)
Ta(1)-C(13)	2.521(10)
Ta(1)-C(15)	2.542(11)
Ta(1)-C(12)	2.563(10)
Ta(1)-C(11)	2.593(11)
S(1)-C(1)	1.801(11)
S(2)-C(4)	1.778(12)
O(1)-C(2)	1.432(13)
O(1)-C(3)	1.451(13)
N(1)-C(21)	1.440(13)
N(1)-C(6)	1.526(13)
N(2)-C(5)	1.313(12)
N(2)-C(31)	1.400(13)
C(1)-C(2)	1.500(17)
C(3)-C(4)	1.462(17)
C(5)-C(6)	1.443(14)
C(6)-C(8)	1.540(15)
C(6)-C(7)	1.551(16)
C(11)-C(15)	1.361(18)
C(11)-C(12)	1.45(2)
C(11)-C(16)	1.518(18)
C(12)-C(13)	1.455(18)
C(12)-C(17)	1.480(19)
C(13)-C(14)	1.358(19)
C(13)-C(18)	1.51(2)
C(14)-C(15)	1.352(18)
C(14)-C(19)	1.57(2)
C(15)-C(20)	1.494(19)
C(21)-C(22)	1.397(16)
C(21)-C(26)	1.418(16)
C(22)-C(23)	1.408(16)
C(22)-C(27)	1.488(18)
C(23)-C(24)	1.338(19)
C(24)-C(25)	1.374(19)
C(25)-C(26)	1.409(15)
C(26)-C(28)	1.481(17)
C(31)-C(36)	1.385(16)
C(31)-C(32)	1.406(16)
C(32)-C(33)	1.350(16)
C(32)-C(37)	1.512(17)
C(33)-C(34)	1.40(2)
C(34)-C(35)	1.40(2)
C(35)-C(36)	1.378(16)

C(36)-C(38)	1.508(17)
N(1)-Ta(1)-C(5)	63.6(4)
N(1)-Ta(1)-O(1)	145.9(3)
C(5)-Ta(1)-O(1)	82.3(3)
N(1)-Ta(1)-S(2)	96.5(3)
C(5)-Ta(1)-S(2)	78.8(3)
O(1)-Ta(1)-S(2)	74.32(18)
N(1)-Ta(1)-S(1)	98.6(3)
C(5)-Ta(1)-S(1)	78.6(3)
O(1)-Ta(1)-S(1)	74.67(18)
S(2)-Ta(1)-S(1)	143.61(10)
N(1)-Ta(1)-C(14)	129.8(4)
C(5)-Ta(1)-C(14)	157.5(4)
O(1)-Ta(1)-C(14)	82.1(4)
S(2)-Ta(1)-C(14)	81.4(4)
S(1)-Ta(1)-C(14)	112.5(4)
N(1)-Ta(1)-C(13)	132.2(4)
C(5)-Ta(1)-C(13)	157.1(4)
O(1)-Ta(1)-C(13)	80.8(3)
S(2)-Ta(1)-C(13)	110.9(3)
S(1)-Ta(1)-C(13)	82.2(3)
C(14)-Ta(1)-C(13)	31.4(4)
N(1)-Ta(1)-C(15)	99.1(4)
C(5)-Ta(1)-C(15)	149.3(4)
O(1)-Ta(1)-C(15)	110.6(4)
S(2)-Ta(1)-C(15)	78.2(3)
S(1)-Ta(1)-C(15)	131.1(3)
C(14)-Ta(1)-C(15)	31.1(4)
C(13)-Ta(1)-C(15)	52.8(4)
N(1)-Ta(1)-C(12)	99.5(4)
C(5)-Ta(1)-C(12)	149.3(4)
O(1)-Ta(1)-C(12)	111.5(4)
S(2)-Ta(1)-C(12)	130.5(3)
S(1)-Ta(1)-C(12)	79.0(3)
C(14)-Ta(1)-C(12)	52.8(4)
C(13)-Ta(1)-C(12)	33.3(4)
C(15)-Ta(1)-C(12)	53.2(4)
N(1)-Ta(1)-C(11)	82.5(3)
C(5)-Ta(1)-C(11)	146.1(4)
O(1)-Ta(1)-C(11)	131.5(3)
S(2)-Ta(1)-C(11)	105.7(4)
S(1)-Ta(1)-C(11)	109.0(4)
C(14)-Ta(1)-C(11)	51.1(4)
C(13)-Ta(1)-C(11)	53.3(4)
C(15)-Ta(1)-C(11)	30.7(4)
C(12)-Ta(1)-C(11)	32.7(4)
C(1)-S(1)-Ta(1)	102.5(4)
C(4)-S(2)-Ta(1)	102.9(4)
C(2)-O(1)-C(3)	112.8(8)
C(2)-O(1)-Ta(1)	123.5(7)
C(3)-O(1)-Ta(1)	122.6(6)
C(21)-N(1)-C(6)	116.0(8)

C(21)-N(1)-Ta(1)	141.5(7)
C(6)-N(1)-Ta(1)	102.6(6)
C(5)-N(2)-C(31)	128.7(9)
C(2)-C(1)-S(1)	111.7(8)
O(1)-C(2)-C(1)	110.0(10)
O(1)-C(3)-C(4)	109.5(9)
C(3)-C(4)-S(2)	112.6(8)
N(2)-C(5)-C(6)	129.3(10)
N(2)-C(5)-Ta(1)	135.4(8)
C(6)-C(5)-Ta(1)	95.2(6)
C(5)-C(6)-N(1)	98.6(8)
C(5)-C(6)-C(8)	116.7(10)
N(1)-C(6)-C(8)	112.2(9)
C(5)-C(6)-C(7)	112.6(9)
N(1)-C(6)-C(7)	111.2(9)
C(8)-C(6)-C(7)	105.6(9)
C(15)-C(11)-C(12)	108.7(11)
C(15)-C(11)-C(16)	126.7(15)
C(12)-C(11)-C(16)	121.5(15)
C(15)-C(11)-Ta(1)	72.6(7)
C(12)-C(11)-Ta(1)	72.5(6)
C(16)-C(11)-Ta(1)	136.6(8)
C(11)-C(12)-C(13)	104.3(11)
C(11)-C(12)-C(17)	129.5(15)
C(13)-C(12)-C(17)	125.0(16)
C(11)-C(12)-Ta(1)	74.8(6)
C(13)-C(12)-Ta(1)	71.8(6)
C(17)-C(12)-Ta(1)	127.7(9)
C(14)-C(13)-C(12)	106.4(11)
C(14)-C(13)-C(18)	130.8(16)
C(12)-C(13)-C(18)	121.5(16)
C(14)-C(13)-Ta(1)	73.5(7)
C(12)-C(13)-Ta(1)	74.9(6)
C(18)-C(13)-Ta(1)	126.8(9)
C(15)-C(14)-C(13)	112.2(12)
C(15)-C(14)-C(19)	123.2(16)
C(13)-C(14)-C(19)	123.8(15)
C(15)-C(14)-Ta(1)	76.1(7)
C(13)-C(14)-Ta(1)	75.1(7)
C(19)-C(14)-Ta(1)	124.3(8)
C(11)-C(15)-C(14)	108.3(12)
C(11)-C(15)-C(20)	125.3(14)
C(14)-C(15)-C(20)	125.0(15)
C(11)-C(15)-Ta(1)	76.7(7)
C(14)-C(15)-Ta(1)	72.8(7)
C(20)-C(15)-Ta(1)	127.5(9)
C(22)-C(21)-C(26)	120.6(10)
C(22)-C(21)-N(1)	120.3(10)
C(26)-C(21)-N(1)	118.9(10)
C(23)-C(22)-C(21)	118.3(11)
C(23)-C(22)-C(27)	116.2(11)
C(21)-C(22)-C(27)	125.4(10)

C(24)-C(23)-C(22)	122.3(12)
C(23)-C(24)-C(25)	119.1(12)
C(24)-C(25)-C(26)	122.9(13)
C(25)-C(26)-C(21)	116.5(11)
C(25)-C(26)-C(28)	118.9(11)
C(21)-C(26)-C(28)	124.6(10)
C(36)-C(31)-N(2)	121.3(10)
C(36)-C(31)-C(32)	118.9(10)
N(2)-C(31)-C(32)	118.9(10)
C(33)-C(32)-C(31)	120.6(12)
C(33)-C(32)-C(37)	117.6(12)
C(31)-C(32)-C(37)	121.8(10)
C(34)-C(33)-C(32)	121.0(14)
C(33)-C(34)-C(35)	118.7(12)
C(36)-C(35)-C(34)	120.2(13)
C(35)-C(36)-C(31)	120.6(12)
C(35)-C(36)-C(38)	116.7(11)
C(31)-C(36)-C(38)	122.6(10)

Table S4''''. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**. 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
Ta(1)	25(1)	26(1)	32(1)	-3(1)	-3(1)	-3(1)
S(1)	30(2)	46(2)	45(2)	1(1)	-9(1)	-5(1)
S(2)	30(2)	46(2)	45(2)	3(1)	-8(1)	-5(1)
O(1)	26(4)	47(4)	37(4)	0(3)	-9(3)	-6(3)
N(1)	29(5)	41(5)	32(5)	0(4)	0(4)	-1(4)
N(2)	43(5)	32(4)	31(5)	-2(4)	-9(4)	-8(4)
C(1)	33(6)	43(6)	41(6)	-4(5)	-8(5)	-2(5)
C(2)	48(8)	70(9)	42(7)	11(6)	-17(6)	-20(7)
C(3)	27(6)	56(7)	50(7)	10(6)	6(5)	-1(5)
C(4)	34(7)	51(7)	59(8)	2(6)	-5(6)	-17(6)
C(5)	29(6)	38(6)	33(6)	4(4)	-14(4)	-3(5)
C(6)	52(7)	28(5)	30(5)	-6(4)	-3(5)	-13(5)
C(7)	56(8)	33(6)	49(7)	-10(5)	8(6)	3(5)
C(8)	70(9)	36(6)	46(7)	-20(5)	3(6)	-23(6)
C(11)	89(11)	25(5)	42(7)	-13(5)	20(7)	-3(6)
C(12)	40(7)	25(5)	100(11)	-11(6)	-4(7)	-18(5)
C(13)	77(10)	28(6)	45(7)	-19(5)	-7(7)	-8(6)
C(14)	61(9)	26(6)	70(9)	-7(6)	15(7)	-3(6)
C(15)	45(7)	31(6)	57(8)	-2(5)	-16(6)	-4(5)
C(16)	210(20)	48(9)	67(11)	-7(7)	44(13)	-51(12)
C(17)	55(10)	43(8)	260(30)	-14(12)	-44(14)	-18(8)
C(18)	230(30)	61(11)	106(15)	15(10)	-93(17)	-44(14)
C(19)	121(17)	42(9)	190(20)	-36(11)	77(16)	-22(10)
C(20)	122(17)	53(9)	156(19)	45(11)	-72(15)	-6(10)
C(21)	43(7)	39(6)	30(6)	-11(4)	-4(5)	-10(5)
C(22)	46(7)	44(6)	40(6)	-15(5)	7(5)	-16(5)
C(23)	45(7)	51(7)	62(9)	-14(6)	17(7)	-19(6)
C(24)	72(10)	69(9)	39(7)	0(6)	10(7)	-24(8)
C(25)	80(10)	54(8)	32(6)	8(5)	-3(6)	-17(7)
C(26)	48(7)	34(6)	39(6)	-14(5)	3(5)	-12(5)
C(27)	50(8)	66(9)	59(8)	-19(7)	0(7)	-17(7)
C(28)	61(9)	61(8)	45(7)	7(6)	-19(6)	-10(7)
C(31)	43(7)	31(5)	38(6)	1(4)	5(5)	-14(5)
C(32)	49(7)	38(6)	39(6)	1(5)	7(5)	-4(5)
C(33)	75(10)	33(6)	64(9)	4(6)	11(8)	-4(7)
C(34)	119(15)	29(6)	71(10)	-3(6)	9(10)	-21(8)
C(35)	76(10)	68(9)	63(9)	-22(7)	-5(8)	-43(9)
C(36)	53(8)	37(6)	48(7)	-9(5)	-5(6)	-19(6)
C(37)	43(7)	49(7)	57(8)	-2(6)	-8(6)	6(6)
C(38)	49(8)	68(9)	56(8)	-7(6)	-12(6)	-30(7)

Table S5^{'''}. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5.

	x	y	z	U(eq)
H(1A)	7952	5085	9537	47
H(1B)	8785	5581	10229	47
H(2A)	5983	5878	10462	63
H(2B)	6765	6883	10375	63
H(3A)	3514	7365	9560	57
H(3B)	3910	6186	9953	57
H(4A)	2407	6517	8648	58
H(4B)	3906	5691	8541	58
H(7A)	10022	5113	7092	57
H(7B)	9926	5069	6019	57
H(7C)	9326	4208	6777	57
H(8A)	6808	4512	6126	58
H(8B)	7450	5344	5354	58
H(8C)	5863	5630	5956	58
H(16A)	8178	8962	5464	129
H(16B)	9375	9410	5964	129
H(16C)	7793	10097	5720	129
H(17A)	10635	8644	7201	138
H(17B)	10389	8238	8278	138
H(17C)	10204	9432	7940	138
H(18A)	7981	9447	9507	153
H(18B)	8237	8233	9677	153
H(18C)	6575	8856	9898	153
H(19A)	3727	9994	8492	144
H(19B)	4276	9170	9333	144
H(19C)	3441	8844	8540	144
H(20A)	5061	9370	5881	135
H(20B)	4410	10242	6516	135
H(20C)	3803	9170	6729	135
H(23)	11744	7531	4354	63
H(24)	10148	8164	3210	72
H(25)	7520	8133	3511	67
H(27A)	10754	6647	6717	68
H(27B)	11818	7418	6149	68
H(27C)	12000	6279	5914	68
H(28A)	5260	8190	4778	67
H(28B)	5445	7365	5674	67
H(28C)	5477	7006	4680	67
H(33)	8693	1484	8581	72
H(34)	6654	914	7989	88
H(35)	4619	2136	7407	77
H(37A)	9038	3290	9422	61
H(37B)	9420	3971	8464	61
H(37C)	10176	2804	8625	61
H(38A)	3530	3812	6937	66
H(38B)	4327	4760	7062	66
H(38C)	3286	4253	7906	66

Table S6'''. Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane) for 5.

Plane 1.

$$1.3612 (0.0492) x + 13.1901 (0.0071) y + 1.8109 (0.0789) z = 14.1354 (0.0732)$$

- * 0.0139 (0.0070) C11
- * -0.0096 (0.0066) C12
- * 0.0023 (0.0068) C13
- * 0.0064 (0.0072) C14
- * -0.0130 (0.0072) C15

Rms deviation of fitted atoms = 0.0100

Plane 2.

$$0.4042 (0.0407) x + 12.6097 (0.0202) y + 5.7125 (0.0652) z = 12.5321 (0.0494)$$

- * -0.0185 (0.0077) C21
- * 0.0306 (0.0078) C22
- * -0.0219 (0.0090) C23
- * -0.0002 (0.0098) C24
- * 0.0130 (0.0091) C25
- * -0.0030 (0.0078) C26

Rms deviation of fitted atoms = 0.0180

Plane 3.

$$- 3.4882 (0.0415) x - 0.2233 (0.0673) y + 12.4132 (0.0384) z = 7.5662 (0.0656)$$

- * 0.0014 (0.0081) C31
- * -0.0088 (0.0083) C32
- * 0.0067 (0.0095) C33
- * 0.0029 (0.0103) C34
- * -0.0102 (0.0099) C35
- * 0.0080 (0.0088) C36

Rms deviation of fitted atoms = 0.0071