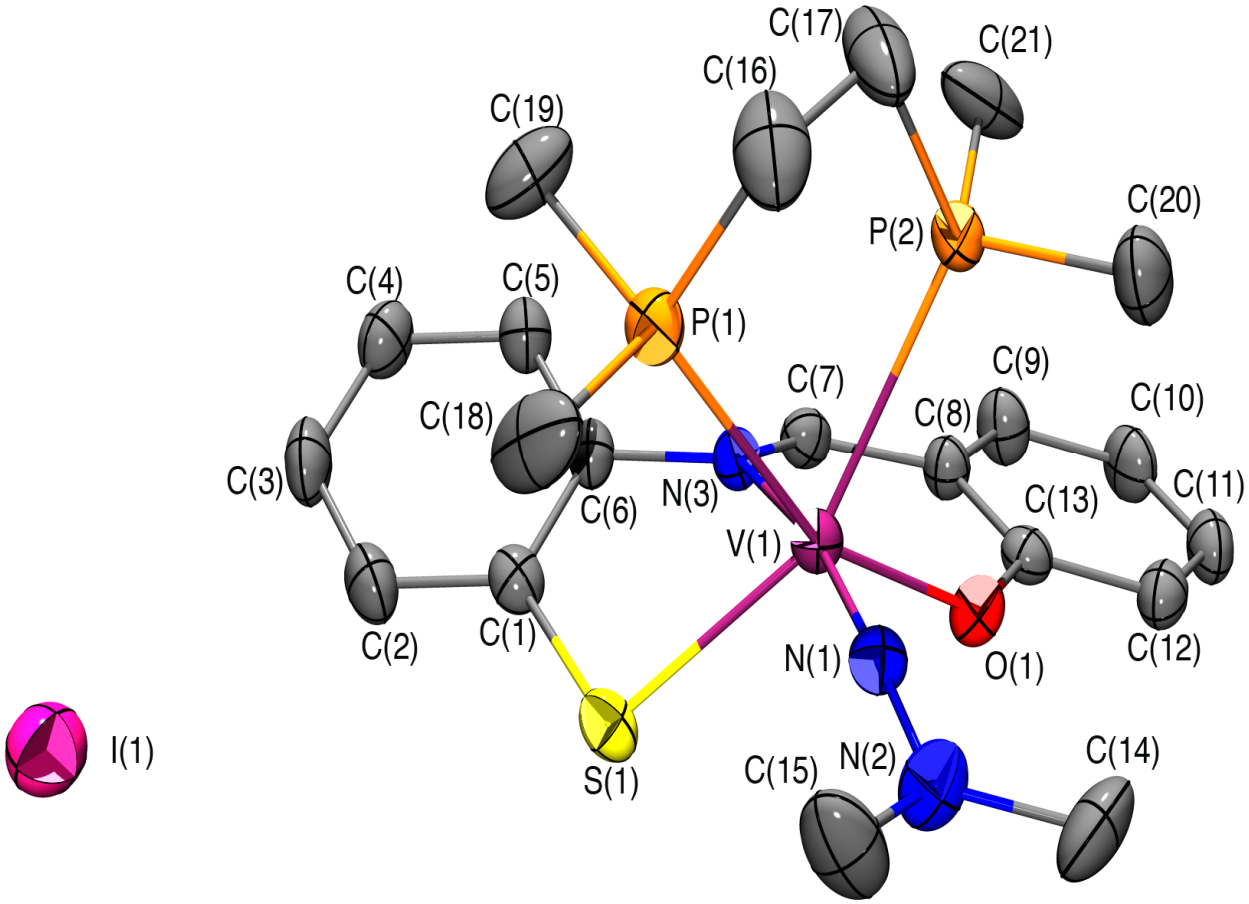

Table 1. Crystal data and structure refinement for odomsb920_0m.

Identification code	odomsb920_0m	
Empirical formula	C21 H31 I N3 O P2 S V	
Formula weight	613.33	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 10.8685(2) Å	α= 90°.
	b = 18.3385(3) Å	β= 90°.
	c = 26.2108(5) Å	γ = 90°.
Volume	5224.13(16) $Å^3$	
Z	8	
Density (calculated)	1.560 Mg/m^3	
Absorption coefficient	1.782 mm^{-1}	
F(000)	2464	
Crystal size	0.28 x 0.12 x 0.10 mm^3	
Theta range for data collection	2.22 to 27.90°.	
Index ranges	-12<=h<=14, -24<=k<=24, -31<=l<=33	
Reflections collected	67170	
Independent reflections	6199 [R(int) = 0.0556]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6199 / 0 / 277	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0325, wR2 = 0.0627	
R indices (all data)	R1 = 0.0566, wR2 = 0.0701	
Largest diff. peak and hole	0.689 and -0.471 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for odomsb920_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
V(1)	7765(1)	4141(1)	3509(1)	22(1)
S(1)	8030(1)	5259(1)	3094(1)	29(1)
P(1)	7387(1)	4955(1)	4262(1)	29(1)
P(2)	7751(1)	3304(1)	4266(1)	29(1)
O(1)	8064(2)	3256(1)	3147(1)	26(1)
N(1)	6231(2)	4125(1)	3388(1)	25(1)
N(2)	5130(2)	4083(1)	3203(1)	36(1)
N(3)	9749(2)	4223(1)	3497(1)	23(1)
C(1)	9483(2)	5494(1)	3342(1)	26(1)
C(2)	9885(3)	6216(1)	3371(1)	33(1)
C(3)	10986(3)	6381(2)	3606(1)	37(1)
C(4)	11702(3)	5833(2)	3814(1)	33(1)
C(5)	11327(2)	5111(1)	3782(1)	28(1)
C(6)	10222(2)	4945(1)	3544(1)	24(1)
C(7)	10530(2)	3710(1)	3392(1)	25(1)
C(8)	10208(2)	2978(1)	3250(1)	24(1)
C(9)	11147(3)	2458(1)	3188(1)	33(1)
C(10)	10898(3)	1769(1)	3015(1)	35(1)
C(11)	9693(3)	1584(1)	2891(1)	32(1)
C(12)	8754(3)	2080(1)	2941(1)	29(1)
C(13)	8990(2)	2786(1)	3121(1)	24(1)
C(14)	4677(3)	3368(2)	3052(1)	51(1)
C(15)	4278(3)	4683(2)	3263(2)	54(1)
C(16)	6605(4)	4428(2)	4757(1)	57(1)
C(17)	7287(4)	3746(2)	4857(1)	65(1)
C(18)	6357(3)	5716(2)	4177(1)	57(1)
C(19)	8688(3)	5351(2)	4581(1)	49(1)
C(20)	6690(3)	2558(2)	4189(1)	43(1)
C(21)	9183(3)	2858(2)	4440(1)	52(1)
I(1)	1920(1)	8379(1)	4394(1)	36(1)

Table 3. Bond lengths [Å] and angles [°] for odomsb920_0m.

V(1)-N(1)	1.698(2)
V(1)-O(1)	1.9081(17)
V(1)-N(3)	2.162(2)
V(1)-S(1)	2.3383(8)
V(1)-P(2)	2.5079(8)
V(1)-P(1)	2.5078(8)
S(1)-C(1)	1.761(3)
P(1)-C(19)	1.796(3)
P(1)-C(18)	1.803(3)
P(1)-C(16)	1.827(3)
P(2)-C(20)	1.801(3)
P(2)-C(21)	1.817(3)
P(2)-C(17)	1.820(3)
O(1)-C(13)	1.328(3)
N(1)-N(2)	1.293(3)
N(2)-C(15)	1.447(4)
N(2)-C(14)	1.455(4)
N(3)-C(7)	1.298(3)
N(3)-C(6)	1.425(3)
C(1)-C(6)	1.393(4)
C(1)-C(2)	1.396(4)
C(2)-C(3)	1.380(4)
C(3)-C(4)	1.382(4)
C(4)-C(5)	1.389(4)
C(5)-C(6)	1.387(4)
C(7)-C(8)	1.437(3)
C(8)-C(9)	1.405(3)
C(8)-C(13)	1.411(4)
C(9)-C(10)	1.370(4)
C(10)-C(11)	1.392(4)
C(11)-C(12)	1.373(4)
C(12)-C(13)	1.402(4)
C(16)-C(17)	1.477(5)

N(1)-V(1)-O(1)	93.40(9)
N(1)-V(1)-N(3)	167.99(9)
O(1)-V(1)-N(3)	83.22(8)
N(1)-V(1)-S(1)	92.79(8)
O(1)-V(1)-S(1)	119.53(6)
N(3)-V(1)-S(1)	79.03(6)
N(1)-V(1)-P(2)	97.55(8)
O(1)-V(1)-P(2)	82.74(6)
N(3)-V(1)-P(2)	93.46(6)
S(1)-V(1)-P(2)	154.89(3)
N(1)-V(1)-P(1)	89.81(8)
O(1)-V(1)-P(1)	157.76(6)
N(3)-V(1)-P(1)	97.69(6)
S(1)-V(1)-P(1)	82.23(3)
P(2)-V(1)-P(1)	75.02(3)
C(1)-S(1)-V(1)	98.82(9)
C(19)-P(1)-C(18)	103.56(17)
C(19)-P(1)-C(16)	104.47(18)
C(18)-P(1)-C(16)	102.08(18)
C(19)-P(1)-V(1)	118.51(11)
C(18)-P(1)-V(1)	117.69(11)
C(16)-P(1)-V(1)	108.62(11)
C(20)-P(2)-C(21)	103.56(16)
C(20)-P(2)-C(17)	104.85(17)
C(21)-P(2)-C(17)	102.90(19)
C(20)-P(2)-V(1)	112.39(11)
C(21)-P(2)-V(1)	117.99(10)
C(17)-P(2)-V(1)	113.73(11)
C(13)-O(1)-V(1)	135.01(16)
N(2)-N(1)-V(1)	168.5(2)
N(1)-N(2)-C(15)	120.3(2)
N(1)-N(2)-C(14)	118.0(2)
C(15)-N(2)-C(14)	119.9(2)
C(7)-N(3)-C(6)	117.1(2)
C(7)-N(3)-V(1)	127.25(17)
C(6)-N(3)-V(1)	115.05(16)

C(6)-C(1)-C(2)	119.0(2)
C(6)-C(1)-S(1)	118.70(19)
C(2)-C(1)-S(1)	122.2(2)
C(3)-C(2)-C(1)	120.3(3)
C(2)-C(3)-C(4)	120.3(3)
C(3)-C(4)-C(5)	120.3(3)
C(6)-C(5)-C(4)	119.4(3)
C(5)-C(6)-C(1)	120.8(2)
C(5)-C(6)-N(3)	123.7(2)
C(1)-C(6)-N(3)	115.5(2)
N(3)-C(7)-C(8)	125.0(2)
C(9)-C(8)-C(13)	119.0(2)
C(9)-C(8)-C(7)	119.1(2)
C(13)-C(8)-C(7)	121.6(2)
C(10)-C(9)-C(8)	121.4(3)
C(9)-C(10)-C(11)	119.2(3)
C(12)-C(11)-C(10)	121.0(3)
C(11)-C(12)-C(13)	120.5(3)
O(1)-C(13)-C(12)	118.6(2)
O(1)-C(13)-C(8)	122.5(2)
C(12)-C(13)-C(8)	118.9(2)
C(17)-C(16)-P(1)	110.0(2)
C(16)-C(17)-P(2)	111.4(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for odomsb920_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
V(1)	19(1)	24(1)	23(1)	0(1)	1(1)	1(1)
S(1)	26(1)	29(1)	33(1)	7(1)	0(1)	4(1)
P(1)	31(1)	29(1)	27(1)	-2(1)	4(1)	4(1)
P(2)	36(1)	27(1)	25(1)	2(1)	1(1)	-5(1)
O(1)	21(1)	29(1)	28(1)	-4(1)	0(1)	2(1)
N(1)	23(1)	29(1)	23(1)	1(1)	1(1)	1(1)
N(2)	19(1)	44(2)	44(2)	-3(1)	-5(1)	-1(1)
N(3)	22(1)	23(1)	25(1)	1(1)	0(1)	0(1)
C(1)	25(1)	29(1)	24(1)	1(1)	7(1)	1(1)
C(2)	39(2)	24(1)	35(2)	3(1)	7(1)	3(1)
C(3)	45(2)	24(1)	41(2)	-2(1)	9(2)	-9(1)
C(4)	29(2)	36(2)	35(2)	-4(1)	1(1)	-6(1)
C(5)	25(2)	28(1)	32(2)	-1(1)	5(1)	0(1)
C(6)	25(1)	22(1)	26(2)	-2(1)	5(1)	-2(1)
C(7)	21(1)	28(1)	26(2)	1(1)	-3(1)	0(1)
C(8)	23(1)	23(1)	27(2)	0(1)	-1(1)	1(1)
C(9)	26(2)	29(1)	42(2)	2(1)	-1(1)	4(1)
C(10)	39(2)	25(2)	40(2)	-1(1)	1(1)	9(1)
C(11)	42(2)	23(1)	31(2)	-2(1)	4(1)	-2(1)
C(12)	31(2)	30(2)	25(2)	-2(1)	3(1)	-5(1)
C(13)	26(1)	26(1)	20(1)	2(1)	2(1)	1(1)
C(14)	44(2)	67(2)	41(2)	-22(2)	0(2)	-19(2)
C(15)	31(2)	55(2)	76(3)	23(2)	-12(2)	7(2)
C(16)	74(3)	49(2)	47(2)	-7(2)	32(2)	-5(2)
C(17)	130(4)	35(2)	30(2)	0(2)	27(2)	-2(2)
C(18)	63(2)	57(2)	50(2)	-21(2)	-11(2)	31(2)
C(19)	37(2)	74(2)	37(2)	-21(2)	0(2)	0(2)
C(20)	42(2)	35(2)	51(2)	5(2)	0(2)	-8(1)
C(21)	40(2)	70(2)	46(2)	34(2)	-6(2)	-7(2)
I(1)	41(1)	40(1)	28(1)	3(1)	0(1)	-11(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for odomsb920_0m.

	x	y	z	U(eq)
H(2)	9410	6587	3230	39
H(3)	11247	6863	3626	44
H(4)	12438	5949	3975	40
H(5)	11812	4742	3919	34
H(7)	11363	3824	3410	30
H(9)	11953	2584	3267	39
H(10)	11528	1429	2980	42
H(11)	9521	1117	2772	38
H(12)	7955	1946	2854	35
H(14A)	5348	3080	2924	76
H(14B)	4068	3423	2790	76
H(14C)	4317	3129	3341	76
H(15A)	3815	4618	3572	81
H(15B)	3726	4695	2977	81
H(15C)	4727	5133	3280	81
H(16A)	6554	4713	5068	68
H(16B)	5775	4313	4647	68
H(17A)	6772	3416	5052	78
H(17B)	8012	3854	5059	78
H(18A)	6279	5977	4492	85
H(18B)	5564	5540	4072	85
H(18C)	6679	6036	3919	85
H(19A)	9032	5729	4372	74
H(19B)	9298	4981	4640	74
H(19C)	8430	5553	4901	74
H(20A)	6735	2244	4481	64
H(20B)	6900	2286	3888	64
H(20C)	5869	2745	4156	64
H(21A)	9072	2596	4754	78
H(21B)	9816	3218	4483	78

H(21C)	9418	2524	4176	78

Table 6. Torsion angles [°] for odomsb920_0m.

N(1)-V(1)-S(1)-C(1)	163.52(11)
O(1)-V(1)-S(1)-C(1)	-100.99(11)
N(3)-V(1)-S(1)-C(1)	-25.34(11)
P(2)-V(1)-S(1)-C(1)	49.06(12)
P(1)-V(1)-S(1)-C(1)	74.10(9)
N(1)-V(1)-P(1)-C(19)	-171.61(16)
O(1)-V(1)-P(1)-C(19)	89.9(2)
N(3)-V(1)-P(1)-C(19)	-1.02(15)
S(1)-V(1)-P(1)-C(19)	-78.77(14)
P(2)-V(1)-P(1)-C(19)	90.52(14)
N(1)-V(1)-P(1)-C(18)	-45.71(17)
O(1)-V(1)-P(1)-C(18)	-144.2(2)
N(3)-V(1)-P(1)-C(18)	124.87(16)
S(1)-V(1)-P(1)-C(18)	47.13(15)
P(2)-V(1)-P(1)-C(18)	-143.58(16)
N(1)-V(1)-P(1)-C(16)	69.51(16)
O(1)-V(1)-P(1)-C(16)	-29.0(2)
N(3)-V(1)-P(1)-C(16)	-119.90(15)
S(1)-V(1)-P(1)-C(16)	162.35(14)
P(2)-V(1)-P(1)-C(16)	-28.36(14)
N(1)-V(1)-P(2)-C(20)	38.93(14)
O(1)-V(1)-P(2)-C(20)	-53.56(13)
N(3)-V(1)-P(2)-C(20)	-136.27(13)
S(1)-V(1)-P(2)-C(20)	152.41(13)
P(1)-V(1)-P(2)-C(20)	126.69(12)
N(1)-V(1)-P(2)-C(21)	159.34(16)
O(1)-V(1)-P(2)-C(21)	66.85(15)
N(3)-V(1)-P(2)-C(21)	-15.86(15)
S(1)-V(1)-P(2)-C(21)	-87.18(16)
P(1)-V(1)-P(2)-C(21)	-112.90(14)
N(1)-V(1)-P(2)-C(17)	-80.01(18)
O(1)-V(1)-P(2)-C(17)	-172.49(18)
N(3)-V(1)-P(2)-C(17)	104.80(18)
S(1)-V(1)-P(2)-C(17)	33.48(19)

P(1)-V(1)-P(2)-C(17)	7.76(17)
N(1)-V(1)-O(1)-C(13)	-165.1(2)
N(3)-V(1)-O(1)-C(13)	26.5(2)
S(1)-V(1)-O(1)-C(13)	99.8(2)
P(2)-V(1)-O(1)-C(13)	-67.9(2)
P(1)-V(1)-O(1)-C(13)	-67.3(3)
O(1)-V(1)-N(1)-N(2)	-45.9(10)
N(3)-V(1)-N(1)-N(2)	27.3(13)
S(1)-V(1)-N(1)-N(2)	74.0(10)
P(2)-V(1)-N(1)-N(2)	-129.0(10)
P(1)-V(1)-N(1)-N(2)	156.2(10)
V(1)-N(1)-N(2)-C(15)	-125.5(9)
V(1)-N(1)-N(2)-C(14)	69.5(11)
N(1)-V(1)-N(3)-C(7)	-89.4(5)
O(1)-V(1)-N(3)-C(7)	-15.1(2)
S(1)-V(1)-N(3)-C(7)	-137.0(2)
P(2)-V(1)-N(3)-C(7)	67.1(2)
P(1)-V(1)-N(3)-C(7)	142.5(2)
N(1)-V(1)-N(3)-C(6)	81.6(5)
O(1)-V(1)-N(3)-C(6)	155.85(18)
S(1)-V(1)-N(3)-C(6)	33.94(16)
P(2)-V(1)-N(3)-C(6)	-121.89(17)
P(1)-V(1)-N(3)-C(6)	-46.56(17)
V(1)-S(1)-C(1)-C(6)	20.3(2)
V(1)-S(1)-C(1)-C(2)	-155.8(2)
C(6)-C(1)-C(2)-C(3)	-1.5(4)
S(1)-C(1)-C(2)-C(3)	174.6(2)
C(1)-C(2)-C(3)-C(4)	0.3(4)
C(2)-C(3)-C(4)-C(5)	0.7(4)
C(3)-C(4)-C(5)-C(6)	-0.5(4)
C(4)-C(5)-C(6)-C(1)	-0.7(4)
C(4)-C(5)-C(6)-N(3)	-179.1(2)
C(2)-C(1)-C(6)-C(5)	1.7(4)
S(1)-C(1)-C(6)-C(5)	-174.5(2)
C(2)-C(1)-C(6)-N(3)	-179.7(2)
S(1)-C(1)-C(6)-N(3)	4.1(3)

C(7)-N(3)-C(6)-C(5)	-40.4(4)
V(1)-N(3)-C(6)-C(5)	147.7(2)
C(7)-N(3)-C(6)-C(1)	141.1(2)
V(1)-N(3)-C(6)-C(1)	-30.8(3)
C(6)-N(3)-C(7)-C(8)	-169.3(2)
V(1)-N(3)-C(7)-C(8)	1.5(4)
N(3)-C(7)-C(8)-C(9)	-174.6(3)
N(3)-C(7)-C(8)-C(13)	11.7(4)
C(13)-C(8)-C(9)-C(10)	-1.0(4)
C(7)-C(8)-C(9)-C(10)	-174.9(3)
C(8)-C(9)-C(10)-C(11)	0.8(4)
C(9)-C(10)-C(11)-C(12)	-0.1(4)
C(10)-C(11)-C(12)-C(13)	-0.3(4)
V(1)-O(1)-C(13)-C(12)	160.11(19)
V(1)-O(1)-C(13)-C(8)	-22.5(4)
C(11)-C(12)-C(13)-O(1)	177.7(2)
C(11)-C(12)-C(13)-C(8)	0.2(4)
C(9)-C(8)-C(13)-O(1)	-176.9(2)
C(7)-C(8)-C(13)-O(1)	-3.2(4)
C(9)-C(8)-C(13)-C(12)	0.5(4)
C(7)-C(8)-C(13)-C(12)	174.2(2)
C(19)-P(1)-C(16)-C(17)	-75.9(3)
C(18)-P(1)-C(16)-C(17)	176.4(3)
V(1)-P(1)-C(16)-C(17)	51.5(3)
P(1)-C(16)-C(17)-P(2)	-44.8(4)
C(20)-P(2)-C(17)-C(16)	-103.4(3)
C(21)-P(2)-C(17)-C(16)	148.6(3)
V(1)-P(2)-C(17)-C(16)	19.8(3)

Symmetry transformations used to generate equivalent atoms:

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