

OHM1552L

SUPPORTING
INFORMATION

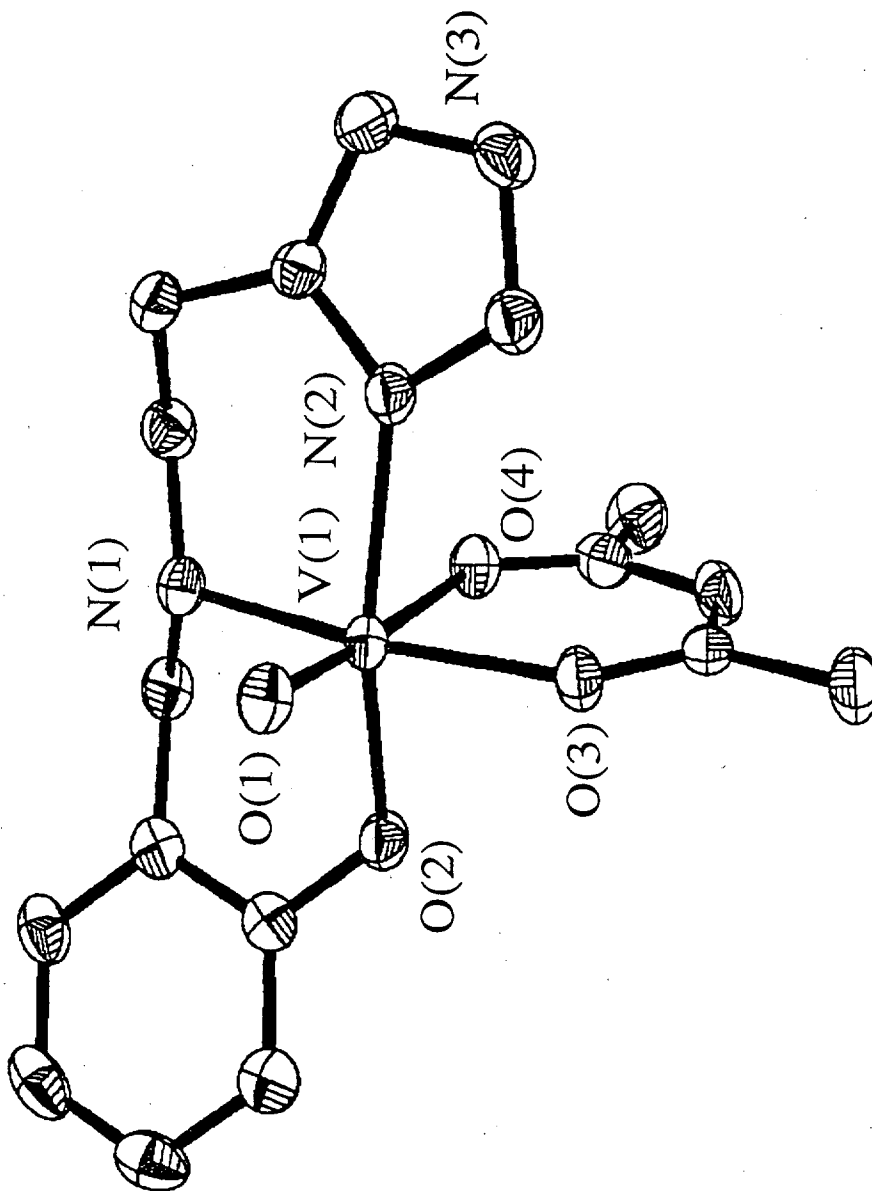


Table 1. Crystal data and structure refinement for TS1.

Identification code	ts1a
Empirical formula	C ₁₇ H ₂₁ N ₃ O ₄ V
Formula weight	382.31
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 7.1004(6) Å alpha = 90 deg. b = 14.1176(11) Å beta = 97.5940(10) deg. c = 17.8887(14) Å gamma = 90 deg.
Volume, Z	1777.4(2) Å ³ , 4
Density (calculated)	1.429 Mg/m ³
Absorption coefficient	0.585 mm ⁻¹
F(000)	796
Crystal size	0.22 x 0.04 x 0.04 mm
Theta range for data collection	1.84 to 25.04 deg.
Limiting indices	-8<=h<=8, -15<=k<=16, -15<=l<=21
Reflections collected	8397
Independent reflections	3117 [R(int) = 0.0540]
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3117 / 0 / 228
Goodness-of-fit on F ²	1.068
Final R indices [I>2sigma(I)]	R1 = 0.0631, wR2 = 0.1315
R indices (all data)	R1 = 0.0871, wR2 = 0.1424
Largest diff. peak and hole	0.703 and -0.284 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TS1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
V(1)	4651(1)	88(1)	1485(1)	20(1)
N(1)	6970(5)	-449(2)	951(2)	23(1)
N(2)	6150(5)	1379(2)	1698(2)	24(1)
N(3)	7004(6)	2737(3)	2231(2)	31(1)
O(1)	3430(4)	404(2)	707(2)	28(1)
O(2)	3650(4)	-1208(2)	1584(2)	27(1)
O(3)	2917(4)	511(2)	2207(2)	26(1)
O(4)	6506(4)	-334(2)	2504(2)	28(1)
C(1)	3694(6)	-1877(3)	1047(2)	26(1)
C(2)	2119(7)	-2449(3)	838(3)	31(1)
C(3)	2158(8)	-3127(3)	273(3)	38(1)
C(4)	3747(8)	-3232(3)	-88(3)	40(1)
C(5)	5342(8)	-2686(3)	137(3)	35(1)
C(6)	5350(7)	-2015(3)	711(2)	27(1)
C(7)	7134(6)	-1497(3)	1004(3)	29(1)
C(8)	8870(6)	-17(3)	1148(3)	30(1)
C(9)	8887(7)	1032(3)	976(3)	30(1)
C(10)	7917(6)	1625(3)	1501(2)	25(1)
C(11)	5679(7)	2071(3)	2136(2)	29(1)
C(12)	8448(7)	2462(3)	1836(3)	30(1)
C(13)	1425(7)	1005(4)	3243(3)	35(1)
C(14)	3079(6)	538(3)	2929(2)	25(1)
C(15)	4597(7)	190(3)	3408(2)	30(1)
C(16)	6211(7)	-251(3)	3181(2)	29(1)
C(17)	7666(7)	-668(4)	3773(3)	40(1)

Table 3. Bond lengths [\AA] for TS1.

V(1)-O(1)	1.603(3)	C(1)-C(2)	1.390(6)
V(1)-O(2)	1.980(3)	C(1)-C(6)	1.404(6)
V(1)-O(3)	1.991(3)	C(2)-C(3)	1.396(7)
V(1)-N(2)	2.119(4)	C(3)-C(4)	1.380(8)
V(1)-N(1)	2.149(4)	C(4)-C(5)	1.385(7)
V(1)-O(4)	2.186(3)	C(5)-C(6)	1.396(6)
N(1)-C(8)	1.480(6)	C(6)-C(7)	1.497(6)
N(1)-C(7)	1.486(5)	C(8)-C(9)	1.514(6)
N(2)-C(11)	1.322(6)	C(9)-C(10)	1.492(6)
N(2)-C(10)	1.392(6)	C(10)-C(12)	1.357(6)
N(3)-C(11)	1.325(6)	C(13)-C(14)	1.517(6)
N(3)-C(12)	1.376(6)	C(14)-C(15)	1.376(6)
O(2)-C(1)	1.349(5)	C(15)-C(16)	1.410(7)
O(3)-C(14)	1.282(5)	C(16)-C(17)	1.499(6)
O(4)-C(16)	1.260(5)		

Table 4. Bond angles [deg] for TS1.

O(1)-V(1)-O(2)	100.10(14)	O(2)-C(1)-C(2)	120.3(4)
O(1)-V(1)-O(3)	99.83(14)	O(2)-C(1)-C(6)	120.1(4)
O(2)-V(1)-O(3)	87.67(12)	C(2)-C(1)-C(6)	119.5(4)
O(1)-V(1)-N(2)	96.8(2)	C(1)-C(2)-C(3)	120.1(5)
O(2)-V(1)-N(2)	163.04(13)	C(4)-C(3)-C(2)	120.5(5)
O(3)-V(1)-N(2)	87.95(13)	C(3)-C(4)-C(5)	119.5(5)
O(1)-V(1)-N(1)	94.03(14)	C(4)-C(5)-C(6)	121.0(5)
O(2)-V(1)-N(1)	91.06(13)	C(5)-C(6)-C(1)	119.2(4)
O(3)-V(1)-N(1)	166.10(13)	C(5)-C(6)-C(7)	120.7(4)
N(2)-V(1)-N(1)	89.27(13)	C(1)-C(6)-C(7)	120.0(4)
O(1)-V(1)-O(4)	175.71(14)	N(1)-C(7)-C(6)	114.1(4)
O(2)-V(1)-O(4)	81.78(12)	N(1)-C(8)-C(9)	112.7(4)
O(3)-V(1)-O(4)	84.07(12)	C(10)-C(9)-C(8)	113.8(4)
N(2)-V(1)-O(4)	81.47(13)	C(12)-C(10)-N(2)	108.2(4)
N(1)-V(1)-O(4)	82.05(12)	C(12)-C(10)-C(9)	130.0(4)
C(8)-N(1)-C(7)	109.5(3)	N(2)-C(10)-C(9)	121.8(4)
C(8)-N(1)-V(1)	118.5(3)	N(2)-C(11)-N(3)	111.7(4)
C(7)-N(1)-V(1)	112.4(3)	C(10)-C(12)-N(3)	106.9(4)
C(11)-N(2)-C(10)	105.9(4)	O(3)-C(14)-C(15)	125.1(4)
C(11)-N(2)-V(1)	125.5(3)	O(3)-C(14)-C(13)	114.5(4)
C(10)-N(2)-V(1)	128.1(3)	C(15)-C(14)-C(13)	120.4(4)
C(11)-N(3)-C(12)	107.4(4)	C(14)-C(15)-C(16)	125.3(4)
C(1)-O(2)-V(1)	122.7(3)	O(4)-C(16)-C(15)	124.2(4)
C(14)-O(3)-V(1)	133.0(3)	O(4)-C(16)-C(17)	117.1(4)
C(16)-O(4)-V(1)	128.1(3)	C(15)-C(16)-C(17)	118.7(4)

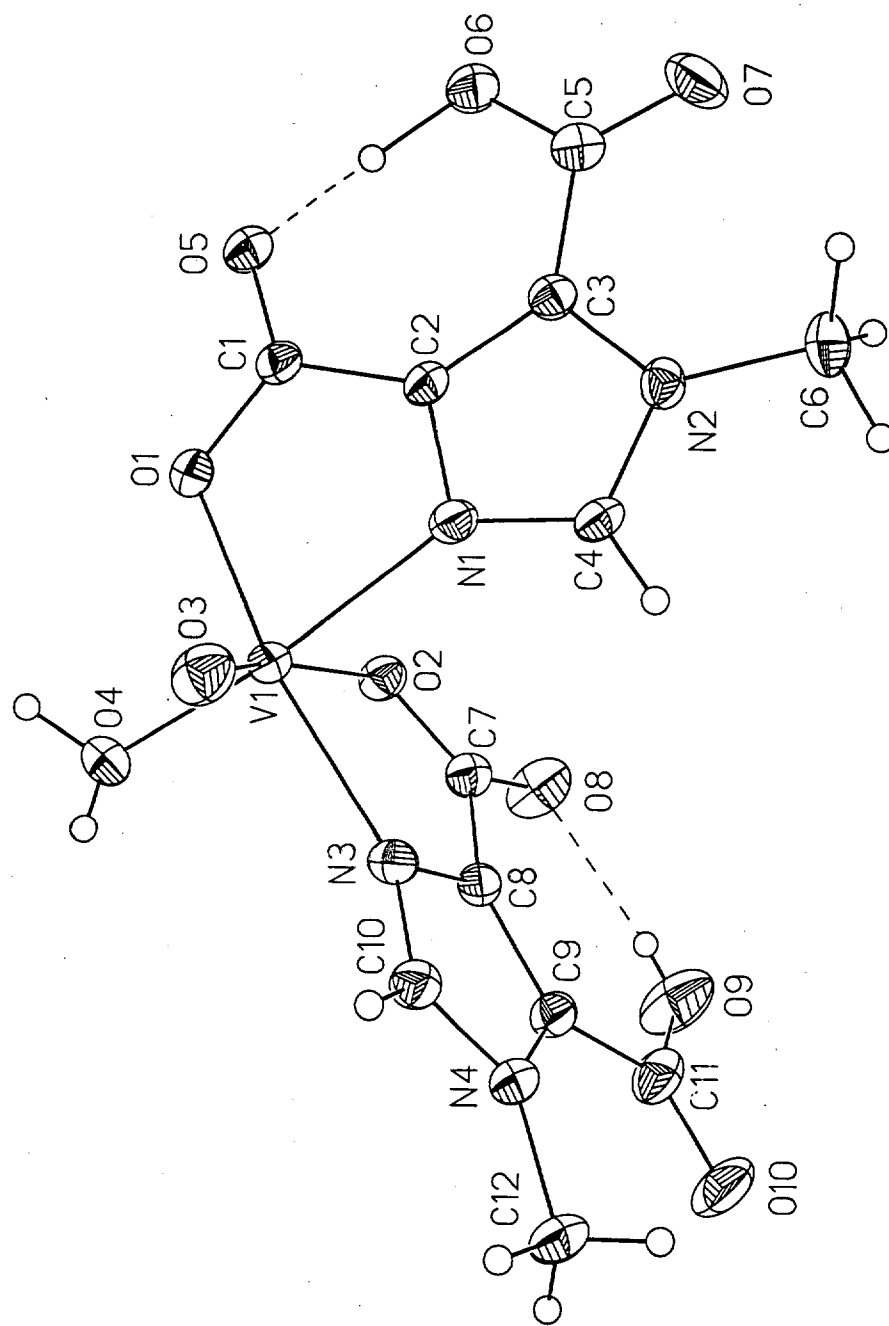
Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TS1. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V(1)	23(1)	21(1)	17(1)	1(1)	5(1)	2(1)
N(1)	23(2)	26(2)	20(2)	3(2)	4(2)	4(2)
N(2)	27(2)	23(2)	22(2)	-2(2)	6(2)	1(2)
N(3)	45(2)	20(2)	29(2)	-3(2)	7(2)	0(2)
O(1)	29(2)	30(2)	24(2)	3(1)	6(1)	4(1)
O(2)	33(2)	22(2)	27(2)	-2(1)	11(1)	-1(1)
O(3)	27(2)	30(2)	20(2)	-4(1)	6(1)	2(1)
O(4)	31(2)	30(2)	22(2)	2(1)	5(1)	3(1)
C(1)	30(3)	22(2)	25(2)	3(2)	1(2)	3(2)
C(2)	35(3)	27(2)	30(3)	6(2)	2(2)	1(2)
C(3)	44(3)	28(3)	40(3)	2(2)	-8(2)	-6(2)
C(4)	62(4)	26(3)	29(3)	-5(2)	-2(3)	-1(3)
C(5)	51(3)	27(3)	28(3)	-4(2)	9(2)	4(2)
C(6)	32(3)	24(2)	26(2)	1(2)	2(2)	4(2)
C(7)	27(2)	28(2)	32(3)	-3(2)	10(2)	9(2)
C(8)	27(2)	32(3)	30(2)	-3(2)	5(2)	2(2)

C(9)	30(3)	32(3)	30(2)	-2(2)	13(2)	-3(2)
C(10)	30(2)	24(2)	21(2)	5(2)	2(2)	-2(2)
C(11)	34(3)	26(2)	27(2)	-1(2)	8(2)	1(2)
C(12)	28(3)	28(3)	33(3)	1(2)	7(2)	-3(2)
C(13)	43(3)	38(3)	28(3)	-6(2)	15(2)	0(2)
C(14)	30(3)	21(2)	27(2)	-4(2)	10(2)	-7(2)
C(15)	46(3)	27(2)	17(2)	-1(2)	8(2)	-2(2)
C(16)	37(3)	26(2)	21(2)	3(2)	-1(2)	-6(2)
C(17)	45(3)	46(3)	30(3)	8(2)	2(2)	0(3)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TS1.

	x	y	z	U(eq)
H(1A)	6646(5)	-326(2)	451(2)	34
H(3A)	6969(6)	3246(3)	2493(2)	37
H(2A)	1037(7)	-2379(3)	1074(3)	37
H(3B)	1105(8)	-3512(3)	139(3)	46
H(4A)	3747(8)	-3666(3)	-480(3)	48
H(5A)	6425(8)	-2767(3)	-98(3)	42
H(7A)	7498(6)	-1669(3)	1528(3)	34
H(7B)	8142(6)	-1702(3)	725(3)	34
H(8A)	9767(6)	-336(3)	869(3)	36
H(8B)	9286(6)	-113(3)	1681(3)	36
H(9A)	10195(7)	1241(3)	998(3)	36
H(9B)	8272(7)	1134(3)	465(3)	36
H(11A)	4556(7)	2088(3)	2350(2)	34
H(12A)	9573(7)	2789(3)	1804(3)	35
H(13A)	254(8)	729(16)	3012(13)	53
H(13B)	1422(27)	1671(5)	3136(16)	53
H(13C)	1551(25)	910(20)	3779(4)	53
H(15A)	4556(7)	250(3)	3923(2)	36
H(17A)	8907(9)	-598(22)	3622(10)	61
H(17B)	7400(29)	-1328(7)	3833(14)	61
H(17C)	7623(35)	-345(17)	4243(5)	61



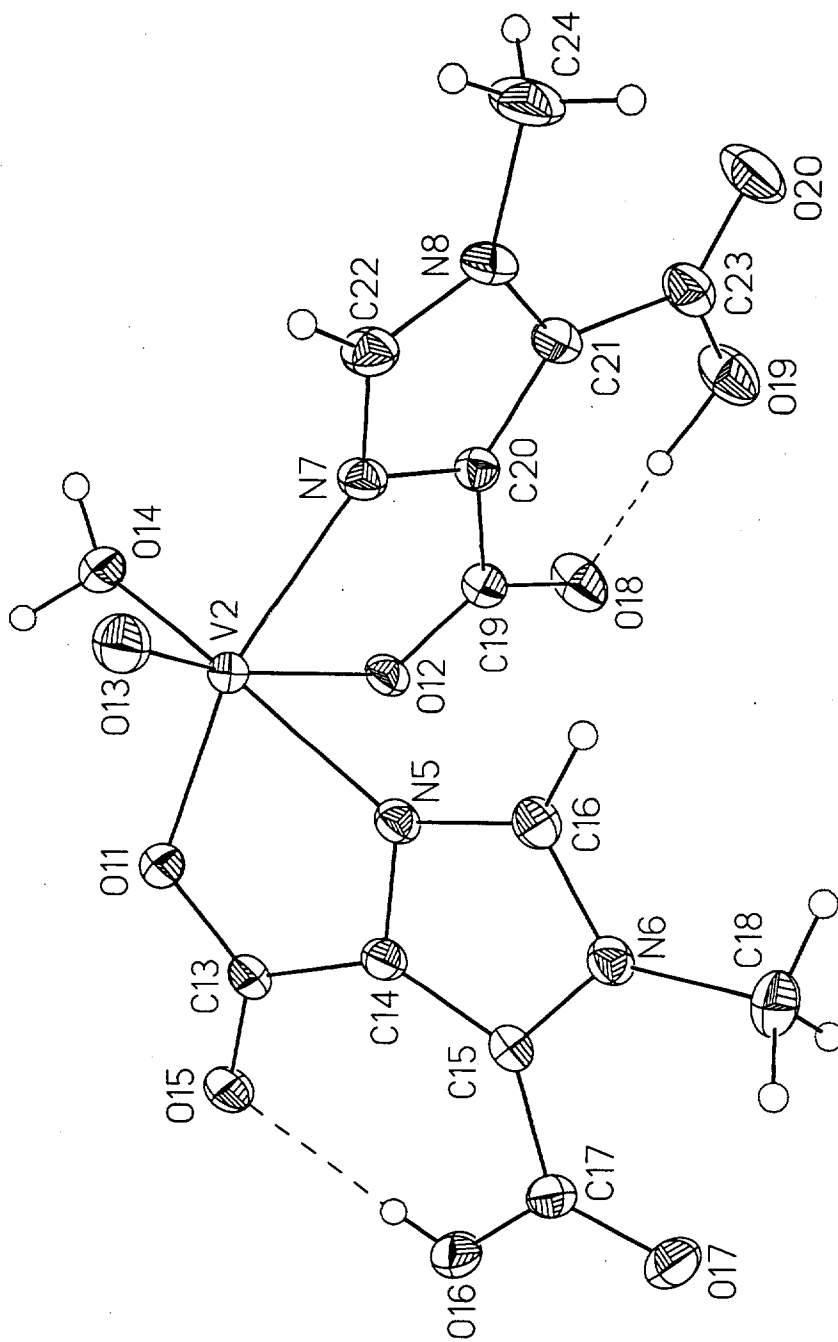


Table 1. Crystal data and structure refinement for 1.

Identification code	vdcbiac
Empirical formula	C12 H15 N4 O11.50 V
Formula weight	450.22
Temperature	158(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	Cc
Unit cell dimensions	a = 27.3557(8) Å alpha = 90 deg. b = 10.2703(2) Å beta = 107.6070(10) deg. c = 13.0845(3) Å gamma = 90 deg.
Volume, Z	3503.9(2) Å ³ , 8
Density (calculated)	1.707 Mg/m ³
Absorption coefficient	0.639 mm ⁻¹
F(000)	1840
Crystal size	0.16 x 0.16 x 0.36 mm
Theta range for data collection	2.13 to 31.62 deg.
Limiting indices	-40<=h<=38, -14<=k<=15, -18<=l<=18
Reflections collected	19344
Independent reflections	9471 [R(int) = 0.0250]
Absorption correction	Sadabs
Max. and min. transmission	0.970 and 0.816
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9454 / 2 / 634
Goodness-of-fit on F ²	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0315, wR2 = 0.0742
R indices (all data)	R1 = 0.0355, wR2 = 0.0773
Absolute structure parameter	0.00
Extinction coefficient	0.00041(8)
Largest diff. peak and hole	0.418 and -0.437 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
V(1)	1804(1)	2464(1)	3776(1)	18(1)
V(2)	58(1)	7896(1)	983(1)	16(1)
N(1)	1909(1)	4353(2)	4362(1)	19(1)
N(2)	2090(1)	6319(2)	5045(2)	18(1)
N(3)	2366(1)	1646(2)	5077(1)	18(1)
N(4)	2862(1)	697(2)	6533(2)	21(1)
N(5)	-3(1)	6002(2)	385(1)	17(1)
N(6)	-213(1)	4048(2)	-296(1)	18(1)
N(7)	-540(1)	8594(2)	-314(1)	18(1)
N(8)	-1071(1)	9413(2)	-1787(2)	23(1)
C(1)	1525(1)	4719(2)	2459(2)	19(1)
C(2)	1752(1)	5247(2)	3550(2)	16(1)
C(3)	1861(1)	6482(2)	3961(2)	18(1)
C(4)	2112(1)	5033(2)	5252(2)	18(1)
C(5)	1768(1)	7761(2)	3422(2)	22(1)
C(6)	2285(1)	7320(2)	5875(2)	25(1)
C(7)	2957(1)	2679(2)	4261(2)	20(1)
C(8)	2870(1)	1901(2)	5151(2)	18(1)
C(9)	3185(1)	1326(2)	6056(2)	20(1)
C(10)	2377(1)	923(2)	5921(2)	21(1)
C(11)	3751(1)	1381(2)	6528(2)	28(1)
C(12)	3008(1)	-146(2)	7492(2)	29(1)
C(13)	366(1)	5648(2)	2292(2)	16(1)
C(14)	138(1)	5109(2)	1201(2)	16(1)
C(15)	15(1)	3877(2)	800(2)	17(1)
C(16)	-214(1)	5329(2)	-506(2)	18(1)
C(17)	80(1)	2599(2)	1329(2)	20(1)
C(18)	-414(1)	3051(2)	-1129(2)	25(1)
C(19)	-1081(1)	7381(2)	515(2)	18(1)
C(20)	-1027(1)	8192(2)	-386(2)	17(1)
C(21)	-1365(1)	8684(2)	-1307(2)	20(1)
C(22)	-580(1)	9327(2)	-1172(2)	22(1)
C(23)	-1928(1)	8464(2)	-1776(2)	26(1)
C(24)	-1245(1)	10222(3)	-2759(2)	35(1)
O(1)	1498(1)	3468(2)	2409(1)	22(1)
O(2)	2555(1)	2962(2)	3524(1)	21(1)
O(3)	1336(1)	2058(2)	4192(1)	29(1)
O(4)	1823(1)	919(2)	2834(2)	25(1)
O(5)	1377(1)	5448(2)	1665(1)	23(1)
O(6)	1587(1)	7776(2)	2376(2)	27(1)
O(7)	1857(1)	8763(2)	3942(2)	34(1)
O(8)	3406(1)	2977(2)	4291(2)	34(1)
O(9)	3996(1)	2039(3)	5977(2)	43(1)
O(10)	3966(1)	884(2)	7386(2)	39(1)
O(11)	399(1)	6895(1)	2337(1)	20(1)
O(12)	-674(1)	7211(1)	1260(1)	19(1)
O(13)	506(1)	8459(2)	568(1)	26(1)
O(14)	-19(1)	9420(2)	1908(1)	23(1)
O(15)	516(1)	4918(2)	3089(1)	22(1)
O(16)	278(1)	2571(2)	2377(2)	25(1)
O(17)	-42(1)	1593(2)	814(1)	27(1)
O(18)	-1517(1)	6948(2)	485(2)	30(1)
O(19)	-2134(1)	7718(2)	-1217(2)	33(1)
O(20)	-2166(1)	8930(2)	-2636(2)	38(1)
O(21)	1167(1)	818(3)	956(2)	48(1)

O(22)	945(1)	3297(2)	-23(2)	39(1)
O(23)	697(1)	9801(2)	3682(2)	38(1)

Table 3. Bond lengths [Å] and angles [deg] for 1.

V(1)-O(3)	1.591(2)
V(1)-O(1)	2.014(2)
V(1)-O(4)	2.020(2)
V(1)-N(1)	2.075(2)
V(1)-N(3)	2.094(2)
V(1)-O(2)	2.236(2)
V(2)-O(13)	1.594(2)
V(2)-O(11)	2.016(2)
V(2)-O(14)	2.029(2)
V(2)-N(5)	2.084(2)
V(2)-N(7)	2.095(2)
V(2)-O(12)	2.251(2)
N(1)-C(4)	1.326(3)
N(1)-C(2)	1.372(2)
N(2)-C(4)	1.346(3)
N(2)-C(3)	1.376(3)
N(2)-C(6)	1.474(3)
N(3)-C(10)	1.322(3)
N(3)-C(8)	1.378(3)
N(4)-C(10)	1.348(3)
N(4)-C(9)	1.384(3)
N(4)-C(12)	1.476(3)
N(5)-C(16)	1.329(3)
N(5)-C(14)	1.371(2)
N(6)-C(16)	1.344(3)
N(6)-C(15)	1.391(3)
N(6)-C(18)	1.475(3)
N(7)-C(22)	1.329(3)
N(7)-C(20)	1.372(3)
N(8)-C(22)	1.345(3)
N(8)-C(21)	1.382(3)
N(8)-C(24)	1.472(3)
C(1)-O(5)	1.245(3)
C(1)-O(1)	1.288(3)
C(1)-C(2)	1.477(3)
C(2)-C(3)	1.374(3)
C(3)-C(5)	1.477(3)
C(5)-O(7)	1.218(3)
C(5)-O(6)	1.307(3)
C(7)-O(8)	1.257(3)
C(7)-O(2)	1.258(3)
C(7)-C(8)	1.490(3)
C(8)-C(9)	1.370(3)
C(9)-C(11)	1.483(3)
C(11)-O(10)	1.212(3)
C(11)-O(9)	1.311(3)
C(13)-O(15)	1.248(3)
C(13)-O(11)	1.284(2)
C(13)-C(14)	1.481(3)
C(14)-C(15)	1.373(3)
C(15)-C(17)	1.470(3)
C(17)-O(17)	1.223(3)
C(17)-O(16)	1.314(3)
C(19)-O(12)	1.252(3)
C(19)-O(18)	1.260(3)
C(19)-C(20)	1.488(3)
C(20)-C(21)	1.375(3)
C(21)-C(23)	1.491(3)
C(23)-O(20)	1.215(3)
C(23)-O(19)	1.300(3)

O(3)-V(1)-O(1)	106.12(8)
O(3)-V(1)-O(4)	100.07(8)
O(1)-V(1)-O(4)	86.59(7)
O(3)-V(1)-N(1)	98.89(8)
O(1)-V(1)-N(1)	79.84(7)
O(4)-V(1)-N(1)	159.14(7)
O(3)-V(1)-N(3)	94.89(8)
O(1)-V(1)-N(3)	158.88(7)
O(4)-V(1)-N(3)	91.88(7)
N(1)-V(1)-N(3)	95.10(7)
O(3)-V(1)-O(2)	168.71(8)
O(1)-V(1)-O(2)	84.53(6)
O(4)-V(1)-O(2)	84.01(7)
N(1)-V(1)-O(2)	79.02(7)
N(3)-V(1)-O(2)	74.36(6)
O(13)-V(2)-O(11)	106.60(8)
O(13)-V(2)-O(14)	98.80(8)
O(11)-V(2)-O(14)	88.46(6)
O(13)-V(2)-N(5)	101.10(8)
O(11)-V(2)-N(5)	79.46(6)
O(14)-V(2)-N(5)	158.98(7)
O(13)-V(2)-N(7)	95.27(8)
O(11)-V(2)-N(7)	157.91(7)
O(14)-V(2)-N(7)	91.29(7)
N(5)-V(2)-N(7)	93.55(7)
O(13)-V(2)-O(12)	169.08(8)
O(11)-V(2)-O(12)	84.06(6)
O(14)-V(2)-O(12)	83.53(6)
N(5)-V(2)-O(12)	78.20(6)
N(7)-V(2)-O(12)	73.96(6)
C(4)-N(1)-C(2)	106.1(2)
C(4)-N(1)-V(1)	142.3(2)
C(2)-N(1)-V(1)	111.31(13)
C(4)-N(2)-C(3)	107.8(2)
C(4)-N(2)-C(6)	123.5(2)
C(3)-N(2)-C(6)	128.7(2)
C(10)-N(3)-C(8)	106.2(2)
C(10)-N(3)-V(1)	136.8(2)
C(8)-N(3)-V(1)	116.98(13)
C(10)-N(4)-C(9)	107.4(2)
C(10)-N(4)-C(12)	124.8(2)
C(9)-N(4)-C(12)	127.6(2)
C(16)-N(5)-C(14)	106.3(2)
C(16)-N(5)-V(2)	141.20(14)
C(14)-N(5)-V(2)	111.11(13)
C(16)-N(6)-C(15)	107.9(2)
C(16)-N(6)-C(18)	123.5(2)
C(15)-N(6)-C(18)	128.6(2)
C(22)-N(7)-C(20)	106.4(2)
C(22)-N(7)-V(2)	136.3(2)
C(20)-N(7)-V(2)	117.18(13)
C(22)-N(8)-C(21)	107.9(2)
C(22)-N(8)-C(24)	123.9(2)
C(21)-N(8)-C(24)	128.1(2)
O(5)-C(1)-O(1)	123.9(2)
O(5)-C(1)-C(2)	121.4(2)
O(1)-C(1)-C(2)	114.7(2)
N(1)-C(2)-C(3)	109.5(2)
N(1)-C(2)-C(1)	116.4(2)
C(3)-C(2)-C(1)	134.1(2)
C(2)-C(3)-N(2)	105.6(2)
C(2)-C(3)-C(5)	130.4(2)
N(2)-C(3)-C(5)	124.0(2)
N(1)-C(4)-N(2)	111.0(2)
O(7)-C(5)-O(6)	121.6(2)

O(7)-C(5)-C(3)	120.6(2)
O(6)-C(5)-C(3)	117.8(2)
O(8)-C(7)-O(2)	126.1(2)
O(8)-C(7)-C(8)	119.5(2)
O(2)-C(7)-C(8)	114.4(2)
C(9)-C(8)-N(3)	109.5(2)
C(9)-C(8)-C(7)	134.4(2)
N(3)-C(8)-C(7)	116.1(2)
C(8)-C(9)-N(4)	105.7(2)
C(8)-C(9)-C(11)	130.4(2)
N(4)-C(9)-C(11)	123.9(2)
N(3)-C(10)-N(4)	111.2(2)
O(10)-C(11)-O(9)	122.6(2)
O(10)-C(11)-C(9)	121.5(2)
O(9)-C(11)-C(9)	115.8(2)
O(15)-C(13)-O(11)	124.1(2)
O(15)-C(13)-C(14)	121.1(2)
O(11)-C(13)-C(14)	114.8(2)
N(5)-C(14)-C(15)	109.9(2)
N(5)-C(14)-C(13)	116.0(2)
C(15)-C(14)-C(13)	134.1(2)
C(14)-C(15)-N(6)	105.1(2)
C(14)-C(15)-C(17)	131.5(2)
N(6)-C(15)-C(17)	123.4(2)
N(5)-C(16)-N(6)	110.9(2)
O(17)-C(17)-O(16)	120.9(2)
O(17)-C(17)-C(15)	121.4(2)
O(16)-C(17)-C(15)	117.7(2)
O(12)-C(19)-O(18)	125.9(2)
O(12)-C(19)-C(20)	114.6(2)
O(18)-C(19)-C(20)	119.5(2)
N(7)-C(20)-C(21)	109.4(2)
N(7)-C(20)-C(19)	116.2(2)
C(21)-C(20)-C(19)	134.3(2)
C(20)-C(21)-N(8)	105.5(2)
C(20)-C(21)-C(23)	129.9(2)
N(8)-C(21)-C(23)	124.5(2)
N(7)-C(22)-N(8)	110.8(2)
O(20)-C(23)-O(19)	123.4(2)
O(20)-C(23)-C(21)	121.2(2)
O(19)-C(23)-C(21)	115.3(2)
C(1)-O(1)-V(1)	117.59(14)
C(7)-O(2)-V(1)	117.62(14)
C(13)-O(11)-V(2)	117.49(13)
C(19)-O(12)-V(2)	117.21(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.
 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
V(1)	16(1)	17(1)	18(1)	2(1)	2(1)	1(1)
V(2)	15(1)	14(1)	17(1)	1(1)	3(1)	-1(1)
N(1)	20(1)	19(1)	16(1)	2(1)	3(1)	3(1)
N(2)	18(1)	20(1)	17(1)	-3(1)	5(1)	0(1)
N(3)	17(1)	18(1)	21(1)	2(1)	6(1)	1(1)
N(4)	23(1)	20(1)	17(1)	3(1)	3(1)	0(1)
N(5)	17(1)	18(1)	14(1)	1(1)	3(1)	1(1)
N(6)	19(1)	20(1)	14(1)	-1(1)	3(1)	1(1)
N(7)	19(1)	18(1)	17(1)	5(1)	5(1)	1(1)
N(8)	26(1)	23(1)	19(1)	7(1)	4(1)	3(1)
C(1)	15(1)	20(1)	20(1)	0(1)	3(1)	2(1)
C(2)	16(1)	19(1)	13(1)	2(1)	3(1)	2(1)
C(3)	16(1)	20(1)	18(1)	1(1)	6(1)	2(1)
C(4)	18(1)	22(1)	14(1)	3(1)	3(1)	4(1)
C(5)	22(1)	22(1)	23(1)	3(1)	7(1)	3(1)
C(6)	29(1)	28(1)	19(1)	-8(1)	7(1)	-3(1)
C(7)	21(1)	20(1)	19(1)	1(1)	6(1)	1(1)
C(8)	17(1)	17(1)	19(1)	-1(1)	4(1)	1(1)
C(9)	19(1)	20(1)	19(1)	1(1)	3(1)	2(1)
C(10)	21(1)	20(1)	22(1)	3(1)	5(1)	-1(1)
C(11)	19(1)	35(1)	25(1)	0(1)	0(1)	2(1)
C(12)	35(1)	29(1)	19(1)	9(1)	0(1)	-1(1)
C(13)	13(1)	21(1)	15(1)	-1(1)	3(1)	2(1)
C(14)	16(1)	16(1)	15(1)	1(1)	3(1)	2(1)
C(15)	15(1)	19(1)	15(1)	1(1)	3(1)	0(1)
C(16)	19(1)	22(1)	14(1)	0(1)	5(1)	0(1)
C(17)	19(1)	16(1)	25(1)	1(1)	6(1)	2(1)
C(18)	27(1)	26(1)	23(1)	-9(1)	7(1)	-5(1)
C(19)	17(1)	20(1)	18(1)	1(1)	6(1)	1(1)
C(20)	17(1)	17(1)	18(1)	1(1)	5(1)	1(1)
C(21)	20(1)	21(1)	18(1)	2(1)	4(1)	3(1)
C(22)	23(1)	22(1)	23(1)	6(1)	8(1)	0(1)
C(23)	20(1)	31(1)	24(1)	-2(1)	2(1)	4(1)
C(24)	39(2)	38(1)	25(1)	18(1)	4(1)	4(1)
O(1)	24(1)	21(1)	17(1)	-2(1)	-1(1)	1(1)
O(2)	22(1)	22(1)	18(1)	3(1)	5(1)	1(1)
O(3)	20(1)	34(1)	31(1)	4(1)	7(1)	0(1)
O(4)	29(1)	17(1)	26(1)	0(1)	5(1)	-3(1)
O(5)	24(1)	24(1)	18(1)	4(1)	2(1)	1(1)
O(6)	31(1)	23(1)	23(1)	6(1)	1(1)	1(1)
O(7)	53(1)	16(1)	33(1)	0(1)	11(1)	4(1)
O(8)	21(1)	51(1)	31(1)	12(1)	10(1)	-2(1)
O(9)	16(1)	67(2)	42(1)	18(1)	5(1)	2(1)
O(10)	28(1)	51(1)	28(1)	8(1)	-7(1)	2(1)
O(11)	21(1)	16(1)	20(1)	-1(1)	2(1)	1(1)
O(12)	19(1)	21(1)	14(1)	3(1)	1(1)	0(1)
O(13)	21(1)	28(1)	30(1)	3(1)	8(1)	-2(1)
O(14)	26(1)	16(1)	23(1)	-1(1)	3(1)	0(1)
O(15)	24(1)	23(1)	14(1)	3(1)	1(1)	2(1)
O(16)	31(1)	17(1)	23(1)	4(1)	1(1)	0(1)
O(17)	35(1)	16(1)	28(1)	-1(1)	6(1)	1(1)
O(18)	17(1)	44(1)	28(1)	10(1)	7(1)	-4(1)
O(19)	18(1)	49(1)	30(1)	7(1)	4(1)	0(1)
O(20)	29(1)	49(1)	28(1)	9(1)	-5(1)	5(1)
O(21)	40(1)	64(2)	37(1)	-13(1)	5(1)	-21(1)

O(22)	25(1)	68(2)	22(1)	9(1)	3(1)	2(1)
O(23)	38(1)	36(1)	31(1)	-4(1)	-3(1)	3(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(4)	2262(12)	4705(28)	5920(26)	30(8)
H(6B)	2580(13)	7788(29)	5731(27)	34(8)
H(10)	2094(11)	609(25)	6094(24)	21(6)
H(12C)	3274(13)	-759(31)	7456(29)	37(9)
H(16)	-349(10)	5700(24)	-1223(22)	15(6)
H(18A)	-639(13)	2507(30)	-887(28)	36(9)
H(18B)	-143(15)	2505(31)	-1159(30)	39(9)
H(18C)	-590(12)	3519(29)	-1802(25)	32(8)
H(22)	-314(11)	9715(24)	-1335(22)	16(6)
H(24A)	-1487(13)	10894(31)	-2652(28)	38(8)
H(24B)	-1414(13)	9693(30)	-3319(30)	34(8)
H(24C)	-937(14)	10574(33)	-2853(30)	46(10)
H(40A)	1796(12)	331(32)	3142(27)	30
H(40B)	1583(18)	913(42)	2199(41)	73(13)
H(60)	1476(19)	6748(47)	2077(38)	81(14)
H(90)	3852(16)	2324(38)	5561(33)	45(12)
H(14A)	234(14)	9483(31)	2523(31)	37(9)
H(14B)	-34(14)	10127(37)	1573(31)	48(10)
H(160)	342(13)	3188(33)	2598(27)	28(9)
H(190)	-1864(13)	7424(30)	-468(29)	40(9)
H(21A)	1023(12)	1418(30)	639(26)	24(8)
H(21B)	919(14)	302(34)	789(29)	41(9)
H(22A)	1054(16)	3943(38)	426(36)	49(10)
H(22B)	830(17)	3743(42)	-484(39)	58(13)
H(23A)	786(15)	10643(43)	3872(34)	64(12)
H(23B)	939(26)	9544(63)	3544(53)	127(25)
H(12B)	2667(14)	-492(33)	7564(30)	47(10)
H(12A)	3180(16)	321(36)	8035(35)	53(11)
H(6A)	2428(12)	6853(29)	6571(25)	31(8)
H(6B)	2004(13)	7911(29)	5873(28)	34(8)

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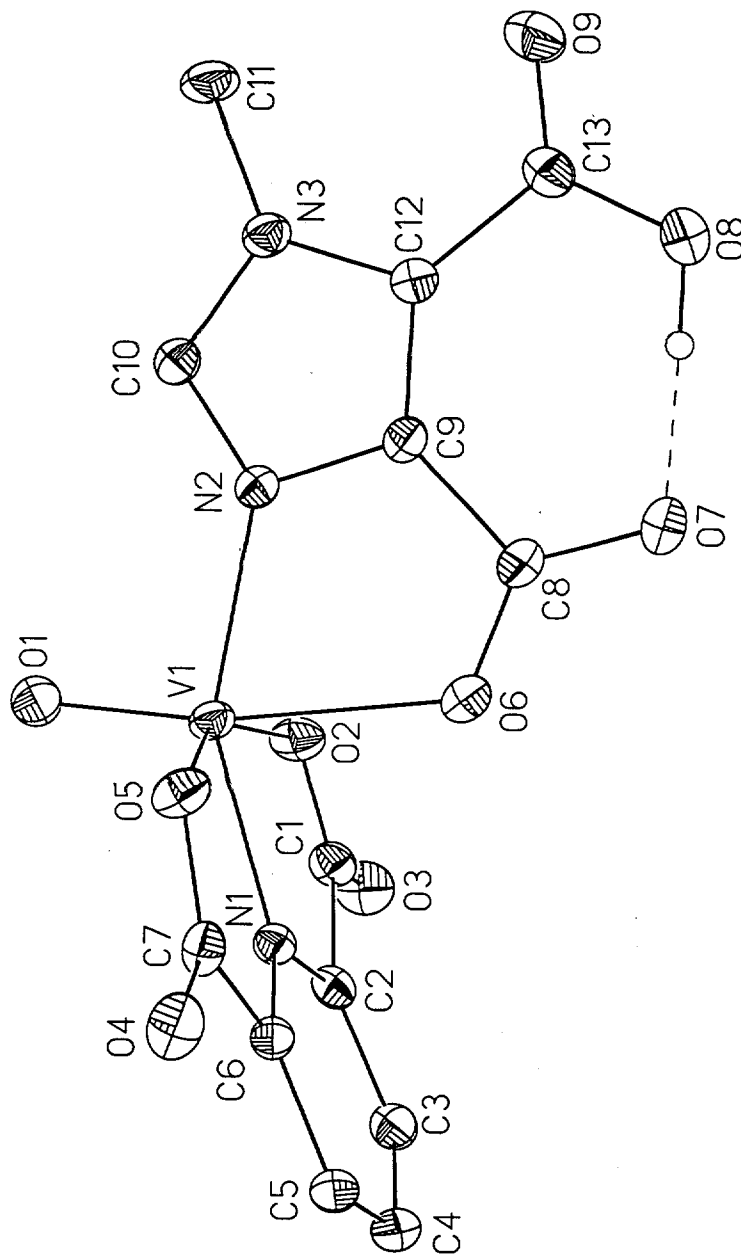


Table 1. Crystal data and structure refinement for 1.

Identification code	vodpc
Empirical formula	C ₂₁ H ₂₈ N ₄ O ₉ V
Formula weight	531.41
Temperature	158(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 7.91940(10) Å alpha = 96.4410(10) deg. b = 10.0286(2) Å beta = 90.5170(10) deg. c = 15.4230(3) Å gamma = 105.7320(10) deg.
Volume, Z	1170.58(4) Å ³ , 2
Density (calculated)	1.508 Mg/m ³
Absorption coefficient	0.483 mm ⁻¹
F(000)	554
Crystal size	0.16 x 0.16 x 0.16 mm
Theta range for data collection	2.64 to 36.38 deg.
Limiting indices	-13<=h<=13, -16<=k<=16, -25<=l<=25
Reflections collected	33348
Independent reflections	10849 [R(int) = 0.0502]
Absorption correction	SADABS
Max. and min. transmission	0.970 and 0.800
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	10718 / 0 / 429
Goodness-of-fit on F ²	1.063
Final R indices [I>2sigma(I)]	R1 = 0.0531, wR2 = 0.0909
R indices (all data)	R1 = 0.0912, wR2 = 0.1046
Extinction coefficient	0.0023(7)
Largest diff. peak and hole	0.473 and -0.388 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
V(1)	8409(1)	4817(1)	1686(1)	16(1)
O(1)	9852(1)	5808(1)	1152(1)	23(1)
O(2)	8480(1)	2922(1)	1124(1)	22(1)
O(3)	7199(2)	1150(1)	96(1)	28(1)
O(4)	4778(1)	7020(1)	1916(1)	22(1)
O(5)	7137(1)	6250(1)	2121(1)	20(1)
O(6)	6726(1)	3597(1)	2695(1)	21(1)
O(7)	6842(1)	2727(1)	3966(1)	27(1)
O(8)	9231(2)	2747(1)	5025(1)	27(1)
O(9)	12125(2)	3614(1)	5239(1)	29(1)
N(1)	6073(1)	4125(1)	1000(1)	14(1)
N(2)	10085(2)	4882(1)	2751(1)	17(1)
N(3)	12282(2)	4993(1)	3671(1)	18(1)
N(4)	1619(2)	-71(1)	2784(1)	18(1)
C(1)	7234(2)	2228(2)	558(1)	19(1)
C(2)	5701(2)	2876(1)	530(1)	16(1)
C(3)	4037(2)	2279(2)	141(1)	19(1)
C(4)	2790(2)	3027(2)	268(1)	20(1)
C(5)	3207(2)	4331(2)	771(1)	18(1)
C(6)	4894(2)	4852(1)	1139(1)	15(1)
C(7)	5628(2)	6168(1)	1766(1)	16(1)
C(8)	7522(2)	3422(1)	3359(1)	19(1)
C(9)	9444(2)	4106(1)	3413(1)	16(1)
C(10)	11798(2)	5407(2)	2931(1)	18(1)
C(11)	14100(2)	5420(2)	4035(1)	25(1)
C(12)	10790(2)	4155(1)	3998(1)	17(1)
C(13)	10779(2)	3489(2)	4812(1)	20(1)
C(14)	142(2)	-1202(2)	3104(1)	23(1)
C(15)	-1322(3)	-714(2)	3535(2)	39(1)
C(16)	2547(2)	983(2)	3542(1)	25(1)
C(17)	3391(3)	403(2)	4239(1)	36(1)
C(18)	916(2)	732(2)	2152(1)	26(1)
C(19)	-92(3)	-152(2)	1358(1)	34(1)
C(20)	2884(2)	-805(2)	2337(1)	19(1)
C(21)	4462(2)	134(2)	1965(1)	27(1)

Table 3. Bond lengths [Å] and angles [deg] for 1.

V(1)-O(1)	1.5992(11)
V(1)-O(2)	2.0142(11)
V(1)-O(5)	2.0273(10)
V(1)-N(1)	2.0311(11)
V(1)-N(2)	2.0870(12)
V(1)-O(6)	2.2963(11)
O(2)-C(1)	1.302(2)
O(3)-C(1)	1.219(2)
O(4)-C(7)	1.228(2)
O(5)-C(7)	1.288(2)
O(6)-C(8)	1.252(2)
O(7)-C(8)	1.266(2)
O(8)-C(13)	1.316(2)
O(9)-C(13)	1.217(2)
N(1)-C(2)	1.332(2)
N(1)-C(6)	1.337(2)
N(2)-C(10)	1.329(2)
N(2)-C(9)	1.370(2)
N(3)-C(10)	1.344(2)
N(3)-C(12)	1.387(2)
N(3)-C(11)	1.473(2)
N(4)-C(16)	1.520(2)
N(4)-C(14)	1.522(2)
N(4)-C(18)	1.522(2)
N(4)-C(20)	1.522(2)
C(1)-C(2)	1.527(2)
C(2)-C(3)	1.390(2)
C(3)-C(4)	1.396(2)
C(4)-C(5)	1.398(2)
C(5)-C(6)	1.386(2)
C(6)-C(7)	1.517(2)
C(8)-C(9)	1.488(2)
C(9)-C(12)	1.378(2)
C(12)-C(13)	1.486(2)
C(14)-C(15)	1.508(2)
C(16)-C(17)	1.510(3)
C(18)-C(19)	1.510(3)
C(20)-C(21)	1.508(2)
O(1)-V(1)-O(2)	100.83(5)
O(1)-V(1)-O(5)	97.19(5)
O(2)-V(1)-O(5)	152.94(4)
O(1)-V(1)-N(1)	111.05(5)
O(2)-V(1)-N(1)	77.54(4)
O(5)-V(1)-N(1)	77.22(4)
O(1)-V(1)-N(2)	95.73(5)
O(2)-V(1)-N(2)	95.79(4)
O(5)-V(1)-N(2)	102.34(4)
N(1)-V(1)-N(2)	153.13(5)
O(1)-V(1)-O(6)	168.21(5)
O(2)-V(1)-O(6)	84.60(4)
O(5)-V(1)-O(6)	81.67(4)
N(1)-V(1)-O(6)	80.24(4)
N(2)-V(1)-O(6)	73.19(4)
C(1)-O(2)-V(1)	118.86(9)
C(7)-O(5)-V(1)	118.79(9)
C(8)-O(6)-V(1)	116.67(9)
C(2)-N(1)-C(6)	122.97(11)
C(2)-N(1)-V(1)	118.18(9)
C(6)-N(1)-V(1)	118.16(9)
C(10)-N(2)-C(9)	106.06(11)

C(10)-N(2)-V(1)	134.81(10)
C(9)-N(2)-V(1)	118.65(9)
C(10)-N(3)-C(12)	107.73(11)
C(10)-N(3)-C(11)	123.33(12)
C(12)-N(3)-C(11)	128.93(12)
C(16)-N(4)-C(14)	110.80(11)
C(16)-N(4)-C(18)	106.99(12)
C(14)-N(4)-C(18)	111.12(12)
C(16)-N(4)-C(20)	110.65(11)
C(14)-N(4)-C(20)	106.55(11)
C(18)-N(4)-C(20)	110.78(11)
O(3)-C(1)-O(2)	126.27(13)
O(3)-C(1)-C(2)	120.67(13)
O(2)-C(1)-C(2)	113.04(12)
N(1)-C(2)-C(3)	120.29(12)
N(1)-C(2)-C(1)	111.55(11)
C(3)-C(2)-C(1)	127.99(12)
C(2)-C(3)-C(4)	117.75(13)
C(3)-C(4)-C(5)	120.91(13)
C(6)-C(5)-C(4)	117.84(12)
N(1)-C(6)-C(5)	120.23(12)
N(1)-C(6)-C(7)	111.44(11)
C(5)-C(6)-C(7)	128.20(12)
O(4)-C(7)-O(5)	125.72(13)
O(4)-C(7)-C(6)	120.42(12)
O(5)-C(7)-C(6)	113.83(11)
O(6)-C(8)-O(7)	126.08(13)
O(6)-C(8)-C(9)	114.99(12)
O(7)-C(8)-C(9)	118.93(13)
N(2)-C(9)-C(12)	109.83(12)
N(2)-C(9)-C(8)	115.95(12)
C(12)-C(9)-C(8)	134.23(13)
N(2)-C(10)-N(3)	111.23(12)
C(9)-C(12)-N(3)	105.15(12)
C(9)-C(12)-C(13)	130.62(13)
N(3)-C(12)-C(13)	124.23(12)
O(9)-C(13)-O(8)	123.00(14)
O(9)-C(13)-C(12)	121.55(14)
O(8)-C(13)-C(12)	115.44(13)
C(15)-C(14)-N(4)	115.73(14)
C(17)-C(16)-N(4)	115.60(14)
C(19)-C(18)-N(4)	114.86(13)
C(21)-C(20)-N(4)	115.44(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.
 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
V(1)	12(1)	16(1)	19(1)	2(1)	-1(1)	4(1)
O(1)	17(1)	27(1)	26(1)	9(1)	2(1)	7(1)
O(2)	20(1)	21(1)	26(1)	0(1)	-3(1)	11(1)
O(3)	32(1)	21(1)	32(1)	-4(1)	-1(1)	14(1)
O(4)	20(1)	16(1)	32(1)	2(1)	7(1)	8(1)
O(5)	16(1)	18(1)	25(1)	-3(1)	-2(1)	4(1)
O(6)	15(1)	23(1)	23(1)	3(1)	-1(1)	1(1)
O(7)	21(1)	29(1)	27(1)	10(1)	2(1)	-3(1)
O(8)	27(1)	28(1)	24(1)	10(1)	0(1)	1(1)
O(9)	27(1)	38(1)	24(1)	9(1)	-4(1)	9(1)
N(1)	14(1)	14(1)	16(1)	2(1)	0(1)	5(1)
N(2)	14(1)	18(1)	18(1)	4(1)	0(1)	3(1)
N(3)	13(1)	21(1)	19(1)	2(1)	0(1)	5(1)
N(4)	19(1)	14(1)	19(1)	0(1)	0(1)	4(1)
C(1)	20(1)	19(1)	21(1)	3(1)	1(1)	9(1)
C(2)	19(1)	15(1)	16(1)	3(1)	0(1)	7(1)
C(3)	22(1)	16(1)	18(1)	1(1)	-2(1)	4(1)
C(4)	16(1)	22(1)	21(1)	4(1)	-4(1)	3(1)
C(5)	15(1)	20(1)	21(1)	5(1)	0(1)	6(1)
C(6)	13(1)	15(1)	17(1)	4(1)	1(1)	5(1)
C(7)	15(1)	14(1)	19(1)	3(1)	4(1)	3(1)
C(8)	16(1)	17(1)	21(1)	1(1)	1(1)	1(1)
C(9)	14(1)	15(1)	18(1)	2(1)	0(1)	3(1)
C(10)	13(1)	21(1)	19(1)	4(1)	1(1)	4(1)
C(11)	14(1)	36(1)	23(1)	4(1)	-4(1)	5(1)
C(12)	16(1)	17(1)	17(1)	1(1)	-1(1)	4(1)
C(13)	25(1)	19(1)	18(1)	2(1)	0(1)	7(1)
C(14)	20(1)	20(1)	26(1)	2(1)	1(1)	0(1)
C(15)	29(1)	39(1)	46(1)	2(1)	15(1)	6(1)
C(16)	25(1)	21(1)	24(1)	-5(1)	1(1)	-1(1)
C(17)	35(1)	41(1)	21(1)	5(1)	-3(1)	-11(1)
C(18)	30(1)	22(1)	30(1)	6(1)	0(1)	13(1)
C(19)	34(1)	45(1)	28(1)	6(1)	-7(1)	18(1)
C(20)	20(1)	15(1)	23(1)	1(1)	1(1)	7(1)
C(21)	25(1)	22(1)	33(1)	5(1)	7(1)	6(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(8O)	8314(37)	2733(28)	4636(18)	65(8)
H(3)	3798(27)	1387(22)	-190(13)	32(5)
H(4)	1646(25)	2639(20)	9(12)	25(5)
H(5)	2388(24)	4821(19)	859(12)	21(4)
H(10)	12573(25)	5973(19)	2593(12)	21(5)
H(11A)	14521(28)	4612(23)	4075(14)	36(6)
H(11B)	14122(27)	5932(22)	4631(14)	34(5)
H(11C)	14785(26)	6062(21)	3656(13)	29(5)
H(14A)	683(26)	-1660(21)	3511(13)	30(5)
H(14B)	-299(26)	-1836(21)	2594(13)	26(5)
H(15A)	-2148(34)	-1546(28)	3714(17)	55(7)
H(15B)	-1952(34)	-314(27)	3157(17)	55(8)
H(15C)	-889(31)	-6(26)	4027(16)	47(7)
H(16A)	1676(27)	1397(21)	3779(13)	30(5)
H(16B)	3419(23)	1672(18)	3288(11)	17(4)
H(17A)	3867(32)	1155(26)	4702(16)	49(7)
H(17B)	4406(31)	44(24)	4020(15)	42(6)
H(17C)	2587(31)	-338(25)	4489(15)	43(6)
H(18A)	161(30)	1194(24)	2495(15)	43(6)
H(18B)	1932(26)	1432(21)	1996(13)	26(5)
H(19A)	-544(32)	435(25)	1025(16)	48(7)
H(19B)	-1117(32)	-899(25)	1513(15)	44(6)
H(19C)	656(31)	-563(24)	994(15)	42(6)
H(20A)	3232(23)	-1316(19)	2777(12)	18(4)
H(20B)	2185(23)	-1475(18)	1881(12)	16(4)
H(21A)	5216(29)	-456(24)	1746(14)	39(6)
H(21B)	5071(29)	843(24)	2369(15)	39(6)
H(21C)	4123(31)	557(25)	1480(16)	47(7)

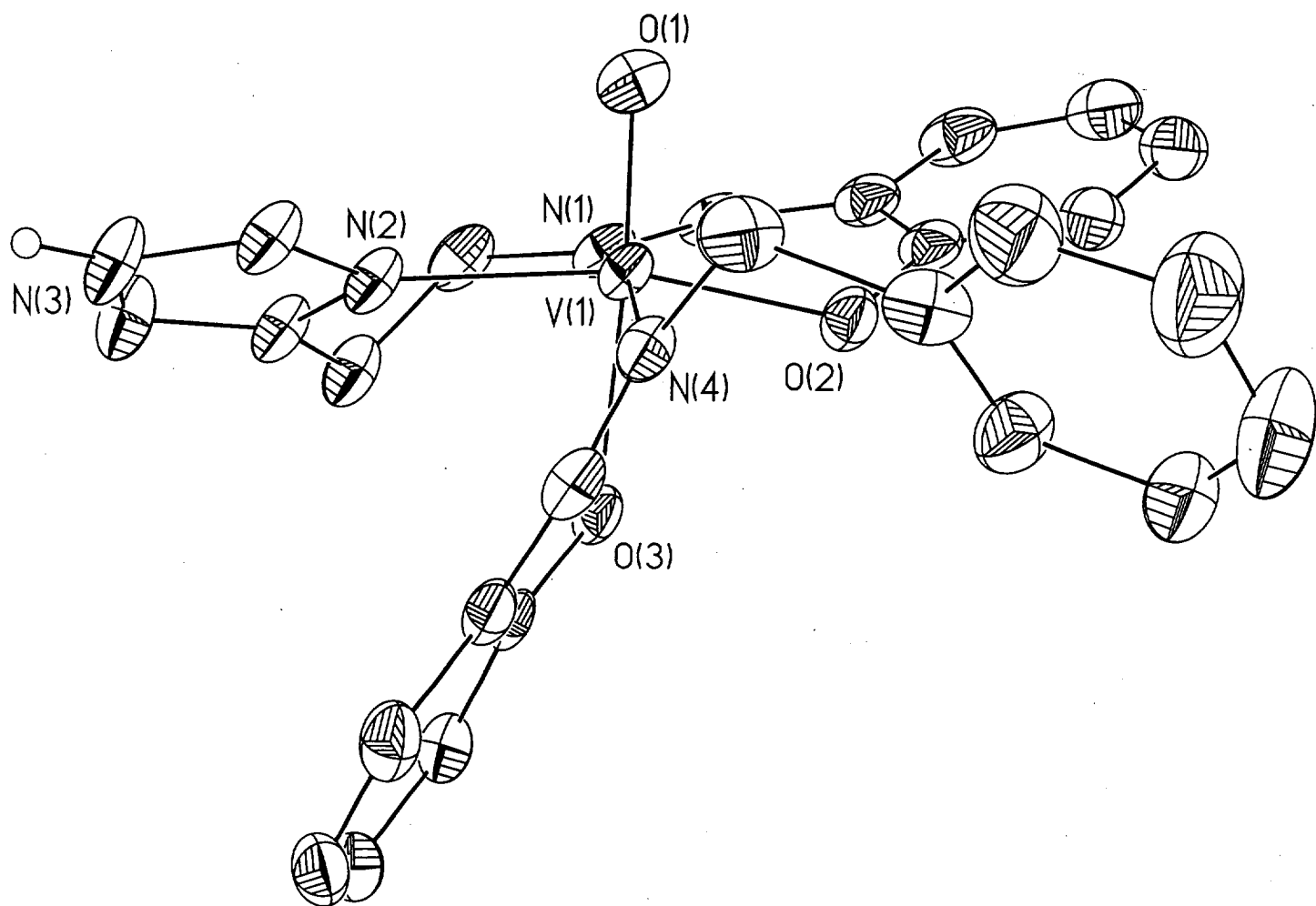


Table 1. Crystal data and structure refinement for vots1.

Identification code	vots1
Empirical formula	C ₂₇ H ₂₈ N ₄ O ₄ V
Formula weight	523.47
Temperature	158(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions deg.	a = 20.4710(3) Å alpha = 90 deg. b = 17.46950(10) Å beta = 109.46 c = 14.77290(10) Å gamma = 90 deg.
Volume	4981.16(9) Å ³
Z, Calculated density	8, 1.396 Mg/m ³
Absorption coefficient	0.439 mm ⁻¹
F(000)	2184
Crystal size	0.06 x 0.16 x 0.20 mm
Theta range for data collection	1.57 to 26.37 deg.
Limiting indices	-25<=h<=25, -21<=k<=21, -18<=l<=18
Reflections collected / unique	44919 / 5100 [R(int) = 0.0519]
Completeness to theta = 26.37	100.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5100 / 0 / 437
Goodness-of-fit on F ²	1.129
Final R indices [I>2sigma(I)]	R1 = 0.0550, wR2 = 0.1110
R indices (all data)	R1 = 0.0696, wR2 = 0.1179
Extinction coefficient	0.00010(8)
Largest diff. peak and hole	0.864 and -0.342 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for vots1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
V(1)	2568(1)	718(1)	9846(1)	24(1)
O(1)	3200(1)	1186(1)	10604(1)	33(1)
O(2)	2849(1)	730(1)	8696(1)	31(1)
O(3)	1750(1)	24(1)	8985(1)	25(1)
N(1)	1915(1)	1664(1)	9260(2)	28(1)
N(2)	2039(1)	565(1)	10846(2)	27(1)
N(3)	1791(1)	251(2)	12137(2)	37(1)
N(4)	3055(1)	-365(1)	10248(2)	27(1)
C(1)	2974(2)	1365(2)	8290(2)	30(1)
C(2)	3506(2)	1362(2)	7873(2)	36(1)
C(3)	3648(2)	2008(2)	7429(2)	42(1)
C(4)	3260(2)	2670(2)	7352(2)	45(1)
C(5)	2733(2)	2686(2)	7738(2)	41(1)
C(6)	2588(2)	2045(2)	8232(2)	32(1)
C(7)	2039(2)	2122(2)	8647(2)	33(1)
C(8)	1332(2)	1892(2)	9594(2)	34(1)
C(9)	944(2)	1215(2)	9827(2)	33(1)
C(10)	1364(1)	790(2)	10714(2)	30(1)
C(11)	1211(2)	595(2)	11515(2)	38(1)
C(12)	2277(2)	244(2)	11716(2)	31(1)
C(13)	1536(1)	-636(2)	9230(2)	24(1)
C(14)	840(2)	-867(2)	8822(2)	29(1)
C(15)	612(2)	-1561(2)	9058(2)	35(1)
C(16)	1070(2)	-2061(2)	9714(2)	35(1)
C(17)	1757(2)	-1852(2)	10109(2)	32(1)
C(18)	2003(1)	-1148(2)	9881(2)	26(1)
C(19)	2743(2)	-1006(2)	10265(2)	27(1)
C(20)	3822(2)	-391(2)	10628(2)	38(1)
C(21)	4152(2)	-760(2)	9924(2)	37(1)
C(22)	3810(2)	-819(2)	8930(2)	41(1)
C(23)	4132(2)	-1168(2)	8346(3)	50(1)
C(24)	4798(2)	-1428(3)	8745(3)	66(1)
C(25)	5153(2)	-1339(3)	9728(3)	70(1)
C(26)	4823(2)	-1019(2)	10312(3)	53(1)
O(4)	611(3)	807(3)	7402(3)	56(1)
C(27)	851(9)	1207(7)	6733(10)	50(3)
O(4A)	298(3)	1875(3)	7229(4)	61(1)
C(27A)	758(9)	1495(10)	6862(13)	73(5)

Table 3. Bond lengths [Å] and angles [deg] for vots1.

V(1)-O(1)	1.622(2)
V(1)-O(2)	1.9667(18)
V(1)-O(3)	2.1154(18)
V(1)-N(2)	2.120(2)
V(1)-N(1)	2.120(2)
V(1)-N(4)	2.130(2)
O(2)-C(1)	1.327(3)
O(3)-C(13)	1.325(3)
N(1)-C(7)	1.296(4)
N(1)-C(8)	1.489(4)
N(2)-C(12)	1.336(3)
N(2)-C(10)	1.385(3)
N(3)-C(12)	1.338(4)
N(3)-C(11)	1.374(4)
N(4)-C(19)	1.293(4)
N(4)-C(20)	1.482(4)
C(1)-C(6)	1.413(4)
C(1)-C(2)	1.418(4)
C(2)-C(3)	1.384(4)
C(3)-C(4)	1.385(5)
C(4)-C(5)	1.379(5)
C(5)-C(6)	1.419(4)
C(6)-C(7)	1.454(4)
C(8)-C(9)	1.527(4)
C(9)-C(10)	1.503(4)
C(10)-C(11)	1.364(4)
C(13)-C(14)	1.409(4)
C(13)-C(18)	1.425(4)
C(14)-C(15)	1.384(4)
C(15)-C(16)	1.406(4)
C(16)-C(17)	1.380(4)
C(17)-C(18)	1.412(4)
C(18)-C(19)	1.452(4)
C(20)-C(21)	1.556(4)
C(21)-C(26)	1.376(5)
C(21)-C(22)	1.405(4)
C(22)-C(23)	1.388(5)
C(23)-C(24)	1.370(6)
C(24)-C(25)	1.399(6)
C(25)-C(26)	1.379(5)
O(4)-C(27)	1.425(16)
O(4A)-C(27A)	1.402(14)
O(1)-V(1)-O(2)	101.28(9)
O(1)-V(1)-O(3)	173.61(9)
O(2)-V(1)-O(3)	83.54(7)
O(1)-V(1)-N(2)	93.31(9)
O(2)-V(1)-N(2)	165.38(8)
O(3)-V(1)-N(2)	81.98(8)
O(1)-V(1)-N(1)	97.98(9)
O(2)-V(1)-N(1)	88.01(8)
O(3)-V(1)-N(1)	86.32(8)
N(2)-V(1)-N(1)	89.09(9)

O(1)-V(1)-N(4)	93.65(9)
O(2)-V(1)-N(4)	90.30(8)
O(3)-V(1)-N(4)	82.05(8)
N(2)-V(1)-N(4)	89.65(8)
N(1)-V(1)-N(4)	168.36(9)
C(1)-O(2)-V(1)	123.76(17)
C(13)-O(3)-V(1)	127.00(15)
C(7)-N(1)-C(8)	115.6(2)
C(7)-N(1)-V(1)	121.5(2)
C(8)-N(1)-V(1)	122.61(18)
C(12)-N(2)-C(10)	106.3(2)
C(12)-N(2)-V(1)	128.05(19)
C(10)-N(2)-V(1)	125.63(17)
C(12)-N(3)-C(11)	107.7(2)
C(19)-N(4)-C(20)	115.8(2)
C(19)-N(4)-V(1)	125.89(19)
C(20)-N(4)-V(1)	118.11(18)
O(2)-C(1)-C(6)	122.8(3)
O(2)-C(1)-C(2)	119.1(3)
C(6)-C(1)-C(2)	118.1(3)
C(3)-C(2)-C(1)	121.1(3)
C(2)-C(3)-C(4)	120.9(3)
C(5)-C(4)-C(3)	119.3(3)
C(4)-C(5)-C(6)	121.5(3)
C(1)-C(6)-C(5)	119.1(3)
C(1)-C(6)-C(7)	123.1(3)
C(5)-C(6)-C(7)	117.8(3)
N(1)-C(7)-C(6)	126.7(3)
N(1)-C(8)-C(9)	113.8(2)
C(10)-C(9)-C(8)	112.9(3)
C(11)-C(10)-N(2)	108.3(2)
C(11)-C(10)-C(9)	130.4(3)
N(2)-C(10)-C(9)	121.2(2)
C(10)-C(11)-N(3)	107.0(3)
N(2)-C(12)-N(3)	110.8(3)
O(3)-C(13)-C(14)	120.8(2)
O(3)-C(13)-C(18)	121.5(2)
C(14)-C(13)-C(18)	117.7(2)
C(15)-C(14)-C(13)	121.5(3)
C(14)-C(15)-C(16)	120.9(3)
C(17)-C(16)-C(15)	118.6(3)
C(16)-C(17)-C(18)	121.6(3)
C(17)-C(18)-C(13)	119.7(3)
C(17)-C(18)-C(19)	117.7(3)
C(13)-C(18)-C(19)	122.4(2)
N(4)-C(19)-C(18)	126.8(3)
N(4)-C(20)-C(21)	113.6(2)
C(26)-C(21)-C(22)	119.4(3)
C(26)-C(21)-C(20)	116.9(3)
C(22)-C(21)-C(20)	123.6(3)
C(23)-C(22)-C(21)	120.5(3)
C(24)-C(23)-C(22)	119.3(4)
C(23)-C(24)-C(25)	120.5(4)
C(26)-C(25)-C(24)	120.1(4)
C(21)-C(26)-C(25)	120.1(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for votsl.
 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
V(1)	31(1)	25(1)	17(1)	-2(1)	8(1)	2(1)
O(1)	37(1)	30(1)	30(1)	-6(1)	8(1)	1(1)
O(2)	45(1)	26(1)	26(1)	-1(1)	18(1)	-3(1)
O(3)	35(1)	26(1)	15(1)	1(1)	11(1)	0(1)
N(1)	38(1)	26(1)	18(1)	-3(1)	5(1)	2(1)
N(2)	31(1)	33(1)	16(1)	-1(1)	6(1)	8(1)
N(3)	47(2)	48(2)	17(1)	4(1)	13(1)	16(1)
N(4)	28(1)	31(1)	22(1)	-3(1)	10(1)	3(1)
C(1)	39(2)	32(2)	16(1)	-2(1)	6(1)	-9(1)
C(2)	40(2)	41(2)	26(1)	0(1)	12(1)	-9(1)
C(3)	50(2)	49(2)	28(2)	0(1)	14(2)	-18(2)
C(4)	69(2)	40(2)	26(2)	2(1)	14(2)	-21(2)
C(5)	60(2)	31(2)	25(2)	0(1)	6(2)	-6(2)
C(6)	44(2)	29(2)	20(1)	-1(1)	6(1)	-7(1)
C(7)	46(2)	24(1)	22(1)	-3(1)	3(1)	1(1)
C(8)	43(2)	34(2)	23(1)	-1(1)	7(1)	12(1)
C(9)	34(2)	45(2)	20(1)	0(1)	8(1)	12(1)
C(10)	33(2)	39(2)	17(1)	-3(1)	8(1)	9(1)
C(11)	38(2)	51(2)	26(1)	3(1)	15(1)	16(1)
C(12)	36(2)	37(2)	17(1)	-1(1)	7(1)	11(1)
C(13)	34(1)	25(1)	17(1)	-3(1)	15(1)	3(1)
C(14)	30(2)	34(2)	26(1)	1(1)	13(1)	5(1)
C(15)	33(2)	40(2)	37(2)	-5(1)	20(1)	-3(1)
C(16)	48(2)	28(2)	41(2)	1(1)	30(2)	-3(1)
C(17)	42(2)	29(2)	29(1)	5(1)	19(1)	6(1)
C(18)	36(2)	26(1)	20(1)	-2(1)	14(1)	2(1)
C(19)	36(2)	27(1)	19(1)	-1(1)	10(1)	9(1)
C(20)	30(2)	37(2)	45(2)	-5(1)	8(1)	6(1)
C(21)	33(2)	31(2)	42(2)	2(1)	6(1)	1(1)
C(22)	31(2)	48(2)	42(2)	-10(2)	10(1)	10(2)
C(23)	59(2)	56(2)	42(2)	-7(2)	27(2)	-6(2)
C(24)	69(3)	83(3)	60(2)	-1(2)	39(2)	23(2)
C(25)	53(2)	101(4)	62(3)	-11(2)	26(2)	13(2)
C(26)	35(2)	73(3)	50(2)	-2(2)	11(2)	6(2)
O(4)	65(3)	73(4)	34(2)	-7(2)	24(2)	-5(3)
C(27)	50(6)	54(7)	40(6)	10(5)	8(5)	0(5)
O(4A)	57(3)	66(3)	58(3)	-2(3)	17(3)	6(3)
C(27A)	44(6)	111(14)	60(7)	-17(9)	10(5)	0(8)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for vots1.

	x	y	z	U(eq)
H(3)	1830(20)	80(20)	12680(30)	63(12)
H(2)	3769(17)	900(20)	7920(20)	46(10)
H(3)	3994(16)	1998(18)	7160(20)	37(9)
H(4)	3355(16)	3120(20)	7050(20)	43(9)
H(5)	2461(17)	3110(20)	7710(20)	39(9)
H(7)	1755(16)	2581(18)	8460(20)	37(8)
H(8A)	1037(17)	2210(20)	9110(20)	45(9)
H(8B)	1534(15)	2237(17)	10180(20)	31(8)
H(9A)	525(16)	1417(18)	9910(20)	37(8)
H(9B)	818(15)	870(18)	9300(20)	34(8)
H(11)	804(17)	640(18)	11660(20)	41(9)
H(12)	2709(15)	10(16)	11990(20)	27(7)
H(14)	517(15)	-560(17)	8400(20)	28(8)
H(15)	117(17)	-1717(18)	8730(20)	38(8)
H(16)	898(16)	-2522(19)	9870(20)	41(9)
H(17)	2075(15)	-2190(18)	10530(20)	32(8)
H(19)	3015(14)	-1462(16)	10526(19)	24(7)
H(20A)	3969	-684	11236	46
H(20B)	4001	138	10777	46
H(22)	3427(19)	-600(20)	8680(30)	50(11)
H(23)	3880(16)	-1207(17)	7730(20)	31(8)
H(24)	5030(20)	-1650(30)	8330(30)	84(14)
H(25)	5710(30)	-1500(30)	10060(40)	130(20)
H(26)	5090(20)	-970(20)	11090(30)	71(12)
H(4A)	937	763	7926	133(18)
H(27A)	630	1712	6603	133(18)
H(27B)	733	915	6134	133(18)
H(27C)	1355	1270	7002	133(18)
H(4A1)	42	1554	7370	133(18)
H(27D)	1070	1868	6724	133(18)
H(27E)	497	1226	6271	133(18)
H(27F)	1031	1125	7337	133(18)

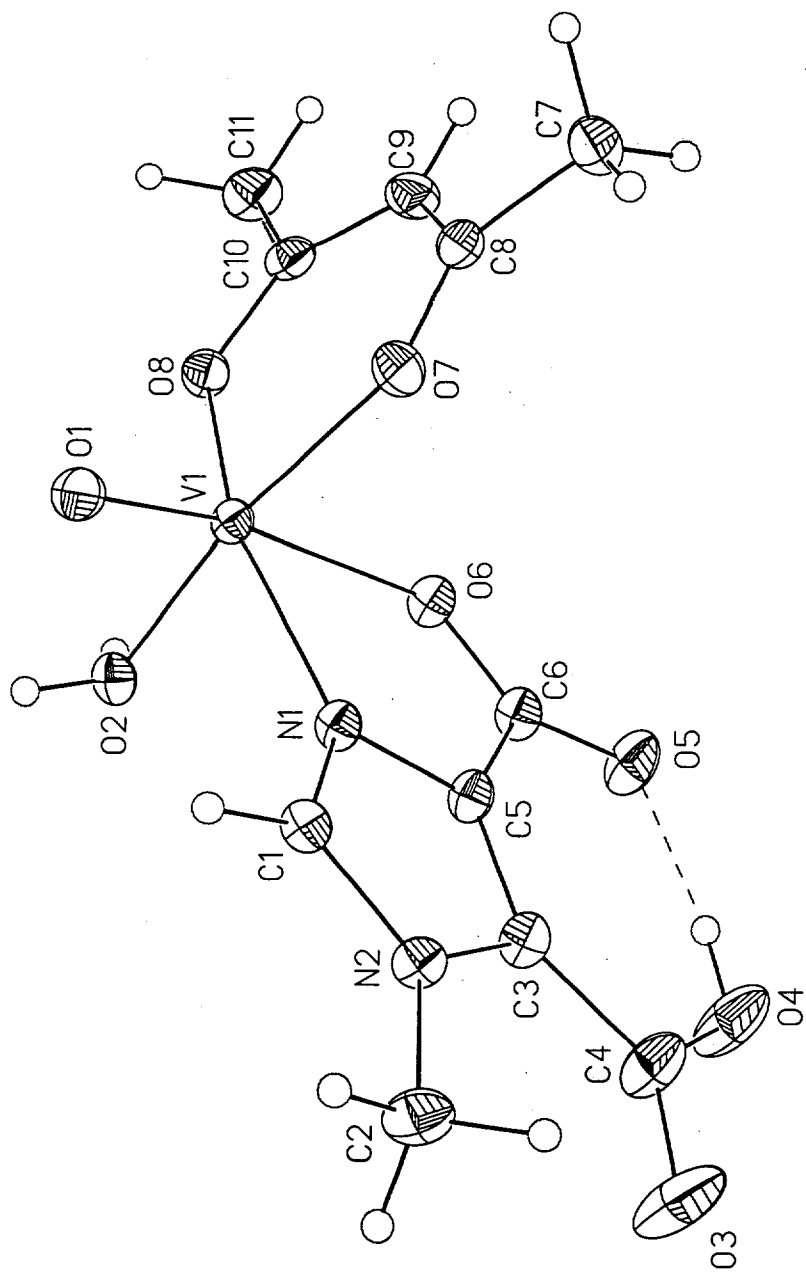


Table 1. Crystal data and structure refinement for 1.

Identification code	ts2
Empirical formula	C11 H14 N2 O8 V
Formula weight	353.18
Temperature	158(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 7.86750(10) Å alpha = 81.8570(10) deg. b = 9.02790(10) Å beta = 85.2040(10) deg. c = 10.88970(10) Å gamma = 67.0390(10) deg.
Volume, Z	704.661(14) Å ³ , 2
Density (calculated)	1.665 Mg/m ³
Absorption coefficient	0.748 mm ⁻¹
F(000)	362
Crystal size	0.44 x 0.32 x 0.22 mm
Theta range for data collection	2.47 to 29.30 deg.
Limiting indices	-10<=h<=10, -11<=k<=12, -14<=l<=14
Reflections collected	8009
Independent reflections	3448 [R(int) = 0.0301]
Absorption correction	SADABS
Max. and min. transmission	0.939 and 0.707
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3448 / 0 / 256
Goodness-of-fit on F ²	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0336, wR2 = 0.0900
R indices (all data)	R1 = 0.0360, wR2 = 0.0913
Largest diff. peak and hole	0.509 and -0.562 e.Å ⁻³
All hydrogen atoms were located on a difference Fourier map and allowed to refine isotropically.	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
V(1)	1688(1)	6325(1)	6067(1)	13(1)
N(1)	1948(2)	4814(2)	7778(1)	15(1)
N(2)	1870(2)	3162(2)	9471(1)	16(1)
O(1)	-392(2)	6507(1)	5854(1)	20(1)
O(2)	2930(2)	4258(1)	5171(1)	16(1)
O(3)	4898(2)	1225(2)	11086(1)	42(1)
O(4)	6709(2)	2368(2)	10039(1)	37(1)
O(5)	6612(2)	4384(2)	8136(1)	25(1)
O(6)	4552(1)	5658(1)	6636(1)	17(1)
O(7)	1133(2)	8216(1)	6987(1)	19(1)
O(8)	2457(2)	7483(1)	4607(1)	18(1)
C(1)	918(2)	4148(2)	8495(1)	15(1)
C(2)	1140(2)	2202(2)	10419(2)	22(1)
C(3)	3631(2)	3196(2)	9378(1)	17(1)
C(4)	5118(2)	2178(2)	10250(2)	27(1)
C(5)	3638(2)	4235(2)	8325(1)	16(1)
C(6)	5072(2)	4786(2)	7666(1)	17(1)
C(7)	1027(3)	10691(2)	7555(2)	25(1)
C(8)	1557(2)	9452(2)	6655(2)	19(1)
C(9)	2430(2)	9734(2)	5518(2)	21(1)
C(10)	2787(2)	8790(2)	4553(2)	18(1)
C(11)	3609(3)	9265(2)	3343(2)	26(1)

Table 3. Bond lengths [Å] and angles [deg] for 1.

V(1)-O(1)	1.6132(11)
V(1)-O(8)	1.9616(11)
V(1)-O(7)	1.9846(11)
V(1)-O(2)	2.0791(11)
V(1)-N(1)	2.1209(13)
V(1)-O(6)	2.2115(11)
N(1)-C(1)	1.331(2)
N(1)-C(5)	1.378(2)
N(2)-C(1)	1.352(2)
N(2)-C(3)	1.392(2)
N(2)-C(2)	1.477(2)
O(3)-C(4)	1.211(2)
O(4)-C(4)	1.325(2)
O(5)-C(6)	1.253(2)
O(6)-C(6)	1.273(2)
O(7)-C(8)	1.282(2)
O(8)-C(10)	1.296(2)
C(3)-C(5)	1.376(2)
C(3)-C(4)	1.489(2)
C(5)-C(6)	1.495(2)
C(7)-C(8)	1.504(2)
C(8)-C(9)	1.406(2)
C(9)-C(10)	1.388(2)
C(10)-C(11)	1.501(2)
O(1)-V(1)-O(8)	107.34(5)
O(1)-V(1)-O(7)	99.29(5)
O(8)-V(1)-O(7)	89.67(5)
O(1)-V(1)-O(2)	94.65(5)
O(8)-V(1)-O(2)	86.53(5)
O(7)-V(1)-O(2)	166.05(5)
O(1)-V(1)-N(1)	94.66(5)
O(8)-V(1)-N(1)	157.80(5)
O(7)-V(1)-N(1)	89.66(5)
O(2)-V(1)-N(1)	88.82(5)
O(1)-V(1)-O(6)	168.42(5)
O(8)-V(1)-O(6)	83.61(4)
O(7)-V(1)-O(6)	84.22(4)
O(2)-V(1)-O(6)	82.02(4)
N(1)-V(1)-O(6)	74.25(4)
C(1)-N(1)-C(5)	106.02(13)
C(1)-N(1)-V(1)	137.19(11)
C(5)-N(1)-V(1)	116.67(10)
C(1)-N(2)-C(3)	107.46(12)
C(1)-N(2)-C(2)	124.72(13)
C(3)-N(2)-C(2)	127.79(13)
C(6)-O(6)-V(1)	119.15(9)
C(8)-O(7)-V(1)	127.27(10)
C(10)-O(8)-V(1)	127.69(10)
N(1)-C(1)-N(2)	111.25(13)
C(5)-C(3)-N(2)	105.38(12)
C(5)-C(3)-C(4)	131.41(14)
N(2)-C(3)-C(4)	123.09(14)
O(3)-C(4)-O(4)	122.3(2)
O(3)-C(4)-C(3)	122.3(2)
O(4)-C(4)-C(3)	115.4(2)
C(3)-C(5)-N(1)	109.89(12)
C(3)-C(5)-C(6)	133.83(14)
N(1)-C(5)-C(6)	116.24(13)
O(5)-C(6)-O(6)	126.20(14)
O(5)-C(6)-C(5)	120.23(14)

O(6)-C(6)-C(5)	113.57(13)
O(7)-C(8)-C(9)	124.83(14)
O(7)-C(8)-C(7)	116.4(2)
C(9)-C(8)-C(7)	118.8(2)
C(10)-C(9)-C(8)	124.26(14)
O(8)-C(10)-C(9)	124.63(14)
O(8)-C(10)-C(11)	115.48(14)
C(9)-C(10)-C(11)	119.90(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.
 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
V(1)	11(1)	15(1)	14(1)	0(1)	-1(1)	-6(1)
N(1)	12(1)	18(1)	15(1)	-2(1)	0(1)	-7(1)
N(2)	14(1)	18(1)	15(1)	-1(1)	2(1)	-7(1)
O(1)	15(1)	20(1)	25(1)	-2(1)	-2(1)	-7(1)
O(2)	14(1)	21(1)	17(1)	-3(1)	2(1)	-9(1)
O(3)	28(1)	58(1)	34(1)	26(1)	-9(1)	-18(1)
O(4)	20(1)	56(1)	32(1)	19(1)	-11(1)	-18(1)
O(5)	16(1)	39(1)	24(1)	5(1)	-5(1)	-14(1)
O(6)	14(1)	22(1)	16(1)	0(1)	1(1)	-10(1)
O(7)	19(1)	19(1)	20(1)	-3(1)	1(1)	-9(1)
O(8)	19(1)	19(1)	17(1)	1(1)	-1(1)	-10(1)
C(1)	13(1)	17(1)	16(1)	-3(1)	1(1)	-6(1)
C(2)	21(1)	24(1)	21(1)	3(1)	4(1)	-11(1)
C(3)	14(1)	22(1)	15(1)	-1(1)	1(1)	-8(1)
C(4)	19(1)	36(1)	22(1)	6(1)	-4(1)	-10(1)
C(5)	12(1)	20(1)	15(1)	-2(1)	0(1)	-6(1)
C(6)	14(1)	22(1)	16(1)	-2(1)	1(1)	-9(1)
C(7)	26(1)	22(1)	29(1)	-7(1)	-5(1)	-8(1)
C(8)	15(1)	17(1)	23(1)	-2(1)	-5(1)	-5(1)
C(9)	23(1)	17(1)	26(1)	2(1)	-2(1)	-11(1)
C(10)	14(1)	18(1)	21(1)	4(1)	-3(1)	-6(1)
C(11)	28(1)	27(1)	23(1)	4(1)	2(1)	-15(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(20A)	3616(38)	4344(31)	4641(25)	40(7)
H(20B)	2229(36)	4017(30)	4864(23)	34(6)
H(4O)	6739(45)	3076(39)	9433(31)	67(10)
H(1)	-371(27)	4332(23)	8340(19)	17(5)
H(2A)	1350(29)	2412(26)	11245(21)	26(5)
H(2B)	1780(31)	1035(28)	10311(22)	32(6)
H(2C)	-178(33)	2557(27)	10321(22)	31(6)
H(7A)	175(45)	11719(40)	7214(31)	68(9)
H(7B)	2075(46)	10738(37)	7775(30)	67(9)
H(7C)	475(42)	10416(37)	8291(30)	61(9)
H(9)	2711(31)	10658(28)	5348(21)	31(6)
H(11A)	4832(36)	8550(30)	3268(23)	38(6)
H(11B)	3725(39)	10278(36)	3331(27)	55(8)
H(11C)	2926(38)	9232(32)	2664(27)	49(8)

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