Inorganic Chemistry
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Table 1. Crystal data and structure refinement for 1.

Identification code	dcccd9m	
Empirical formula	$C_5H_{16}NNa_2O_{13}PV$	
Formula weight	426.08	
Temperature	161(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 10.56320(10) Å	alpha = 90°
	b = 11.18680(10) Å	beta = 106.45°
	c = 12.69210(10) Å	gamma = 90°
Volume, Z	1438.44(2) $Å^3$, 4	
Density (calculated)	1.967 Mg/m^3	
Absorption coefficient	0.932 mm^{-1}	
F(000)	868	
Crystal size	0.58 x 0.26 x 0.26 mm	
θ range for data collection	2.22 to 28.19°	
Limiting indices	$-13 \le h \le 12$, $-14 \le k \le 11$, $-16 \le l \le 12$	
Reflections collected	9337	
Independent reflections	3436 (R_{int} = 0.0388)	
Absorption correction	SADABS Tmax=0.96 Tmin=0.68	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3436 / 0 / 209	
Goodness-of-fit on F^2	1.140	
Final R indices [I>2σ(I)]	R1 = 0.0781, wR2 = 0.1975	
R indices (all data)	R1 = 0.0845, wR2 = 0.2017	
Extinction coefficient	0.003(2)	
Largest diff. peak and hole	1.412 and -0.986 $eÅ^{-3}$	

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

V(1)-O(11)	1.608(4)	V(1)-O(16)	1.985(3)
V(1)-O(17)	2.006(3)	V(1)-O(12)	2.033(4)
V(1)-O(14)	2.065(3)	V(1)-N(1)	2.362(4)
N(1)-C(13)	1.485(6)	N(1)-C(11)	1.487(6)
N(1)-C(15)	1.489(6)	P(1)-O(18)	1.505(3)
P(1)-O(17)#1	1.541(3)	P(1)-O(16)	1.556(3)
P(1)-C(15)	1.833(5)	C(11)-C(12)	1.523(9)
C(12)-O(13)	1.224(7)	C(12)-O(12)	1.296(8)
C(13)-C(14)	1.517(7)	C(14)-O(15)	1.264(6)
C(14)-O(14)	1.275(7)	O(13)-Na(1)#2	2.428(6)
O(13)-Na(2)#3	2.524(5)	O(17)-P(1)#1	1.541(3)
O(18)-Na(2)	2.321(4)	O(18)-Na(1)	2.360(4)
Na(1)-W(3)	2.313(5)	Na(1)-W(1)	2.385(6)
Na(1)-O(13)#4	2.428(6)	Na(1)-W(2)	2.442(6)
Na(1)-W(5)	2.519(10)	Na(1)-Na(2)#5	3.290(4)
Na(1)-Na(2)	3.358(4)	Na(2)-W(2)#6	2.315(5)
Na(2)-W(1)	2.506(6)	Na(2)-W(4)	2.506(8)
Na(2)-W(4)#7	2.539(9)	Na(2)-O(13)#8	2.524(5)
Na(2)-W(3)#6	2.580(5)	Na(2)-Na(1)#6	3.290(4)
W(2)-Na(2)#5	2.315(5)	W(3)-Na(2)#5	2.580(5)
W(4)-Na(2)#7	2.539(9)	W(5)-W(5)#9	1.28(3)
O(11)-V(1)-O(16)	105.9(2)	O(11)-V(1)-O(17)	101.2(2)
O(16)-V(1)-O(17)	89.33(13)	O(11)-V(1)-O(12)	100.4(2)
O(16)-V(1)-O(12)	153.6(2)	O(17)-V(1)-O(12)	87.8(2)
O(11)-V(1)-O(14)	93.0(2)	O(16)-V(1)-O(14)	85.22(14)
O(17)-V(1)-O(14)	165.8(2)	O(12)-V(1)-O(14)	91.2(2)
O(11)-V(1)-N(1)	167.6(2)	O(16)-V(1)-N(1)	79.38(14)
O(17)-V(1)-N(1)	89.9(2)	O(12)-V(1)-N(1)	74.4(2)
O(14)-V(1)-N(1)	76.2(2)	C(13)-N(1)-C(11)	111.5(4)
C(13)-N(1)-C(15)	112.2(4)	C(11)-N(1)-C(15)	112.5(4)
C(13)-N(1)-V(1)	107.6(3)	C(11)-N(1)-V(1)	103.8(3)
C(15)-N(1)-V(1)	108.8(3)	O(18)-P(1)-O(17)#1	111.8(2)
O(18)-P(1)-O(16)	112.2(2)	O(17)#1-P(1)-O(16)	109.2(2)
O(18)-P(1)-C(15)	110.9(2)	O(17)#1-P(1)-C(15)	109.6(2)
O(16)-P(1)-C(15)	102.8(2)	N(1)-C(11)-C(12)	109.9(5)
O(13)-C(12)-O(12)	123.2(6)	O(13)-C(12)-C(11)	120.9(6)
O(12)-C(12)-C(11)	115.9(5)	N(1)-C(13)-C(14)	112.8(4)
O(15)-C(14)-O(14)	122.9(5)	O(15)-C(14)-C(13)	118.8(5)
O(14)-C(14)-C(13)	118.3(4)	N(1)-C(15)-P(1)	108.7(3)
C(12)-O(12)-V(1)	122.6(4)	C(12)-O(13)-Na(1)#2	130.4(5)
C(12)-O(13)-Na(2)#3	145.2(6)	Na(1)#2-O(13)-Na(2)#3	83.2(2)
C(14)-O(14)-V(1)	122.4(3)	P(1)-O(16)-V(1)	126.7(2)
P(1)#1-O(17)-V(1)	137.3(2)	P(1)-O(18)-Na(2)	128.8(2)
P(1)-O(18)-Na(1)	127.2(2)	Na(2)-O(18)-Na(1)	91.65(14)
W(3)-Na(1)-O(18)	94.0(2)	W(3)-Na(1)-W(1)	100.4(2)
O(18)-Na(1)-W(1)	91.9(2)	W(3)-Na(1)-O(13)#4	83.7(2)
O(18)-Na(1)-O(13)#4	164.8(2)	W(1)-Na(1)-O(13)#4	103.3(2)
W(3)-Na(1)-W(2)	82.5(2)	O(18)-Na(1)-W(2)	88.14(14)
W(1)-Na(1)-W(2)	177.2(2)	O(13)#4-Na(1)-W(2)	76.7(2)
W(3)-Na(1)-W(5)	156.5(5)	O(18)-Na(1)-W(5)	96.9(4)
W(1)-Na(1)-W(5)	100.0(4)	O(13)#4-Na(1)-W(5)	80.4(4)
W(2)-Na(1)-W(5)	77.1(4)	W(3)-Na(1)-Na(2)#5	51.30(13)
O(18)-Na(1)-Na(2)#5	118.03(12)	W(1)-Na(1)-Na(2)#5	137.3(2)

O(13)#4-Na(1)-Na(2)#5	49.63(13)	W(2)-Na(1)-Na(2)#5	44.67(12)
W(5)-Na(1)-Na(2)#5	105.3(4)	W(3)-Na(1)-Na(2)	100.7(2)
O(18)-Na(1)-Na(2)	43.71(10)	W(1)-Na(1)-Na(2)	48.2(2)
O(13)#4-Na(1)-Na(2)	151.5(2)	W(2)-Na(1)-Na(2)	131.75(13)
W(5)-Na(1)-Na(2)	101.5(4)	Na(2)#5-Na(1)-Na(2)	149.65(11)
W(2)#6-Na(2)-O(18)	158.6(2)	W(2)#6-Na(2)-W(1)	87.2(2)
O(18)-Na(2)-W(1)	89.8(2)	W(2)#6-Na(2)-W(4)	117.9(2)
O(18)-Na(2)-W(4)	82.0(2)	W(1)-Na(2)-W(4)	77.8(3)
W(2)#6-Na(2)-W(4)#7	88.4(2)	O(18)-Na(2)-W(4)#7	110.4(2)
W(1)-Na(2)-W(4)#7	124.9(3)	W(4)-Na(2)-W(4)#7	56.6(4)
W(2)#6-Na(2)-O(13)#8	77.1(2)	O(18)-Na(2)-O(13)#8	98.9(2)
W(1)-Na(2)-O(13)#8	157.4(2)	W(4)-Na(2)-O(13)#8	124.0(3)
W(4)#7-Na(2)-O(13)#8	71.5(2)	W(2)#6-Na(2)-W(3)#6	79.4(2)
O(18)-Na(2)-W(3)#6	79.2(2)	W(1)-Na(2)-W(3)#6	84.6(2)
W(4)-Na(2)-W(3)#6	154.2(3)	W(4)#7-Na(2)-W(3)#6	147.7(3)
O(13)#8-Na(2)-W(3)#6	76.6(2)	W(2)#6-Na(2)-Na(1)#6	47.86(14)
O(18)-Na(2)-Na(1)#6	114.42(13)	W(1)-Na(2)-Na(1)#6	110.26(14)
W(4)-Na(2)-Na(1)#6	161.0(2)	W(4)#7-Na(2)-Na(1)#6	106.6(2)
O(13)#8-Na(2)-Na(1)#6	47.13(14)	W(3)#6-Na(2)-Na(1)#6	44.38(13)
W(2)#6-Na(2)-Na(1)	128.5(2)	O(18)-Na(2)-Na(1)	44.64(11)
W(1)-Na(2)-Na(1)	45.16(13)	W(4)-Na(2)-Na(1)	76.2(2)
W(4)#7-Na(2)-Na(1)	131.0(2)	O(13)#8-Na(2)-Na(1)	139.0(2)
W(3)#6-Na(2)-Na(1)	78.01(13)	Na(1)#6-Na(2)-Na(1)	121.90(8)
Na(1)-W(1)-Na(2)	86.7(2)	Na(2)#5-W(2)-Na(1)	87.5(2)
Na(1)-W(3)-Na(2)#5	84.3(2)	Na(2)-W(4)-Na(2)#7	123.4(4)
W(5)#9-W(5)-Na(1)	153(2)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z   #2 x+1,y,z   #3 -x+3/2,y-1/2,-z+1/2

#4 x-1,y,z   #5 -x+1/2,y-1/2,-z+1/2   #6 -x+1/2,y+1/2,-z+1/2

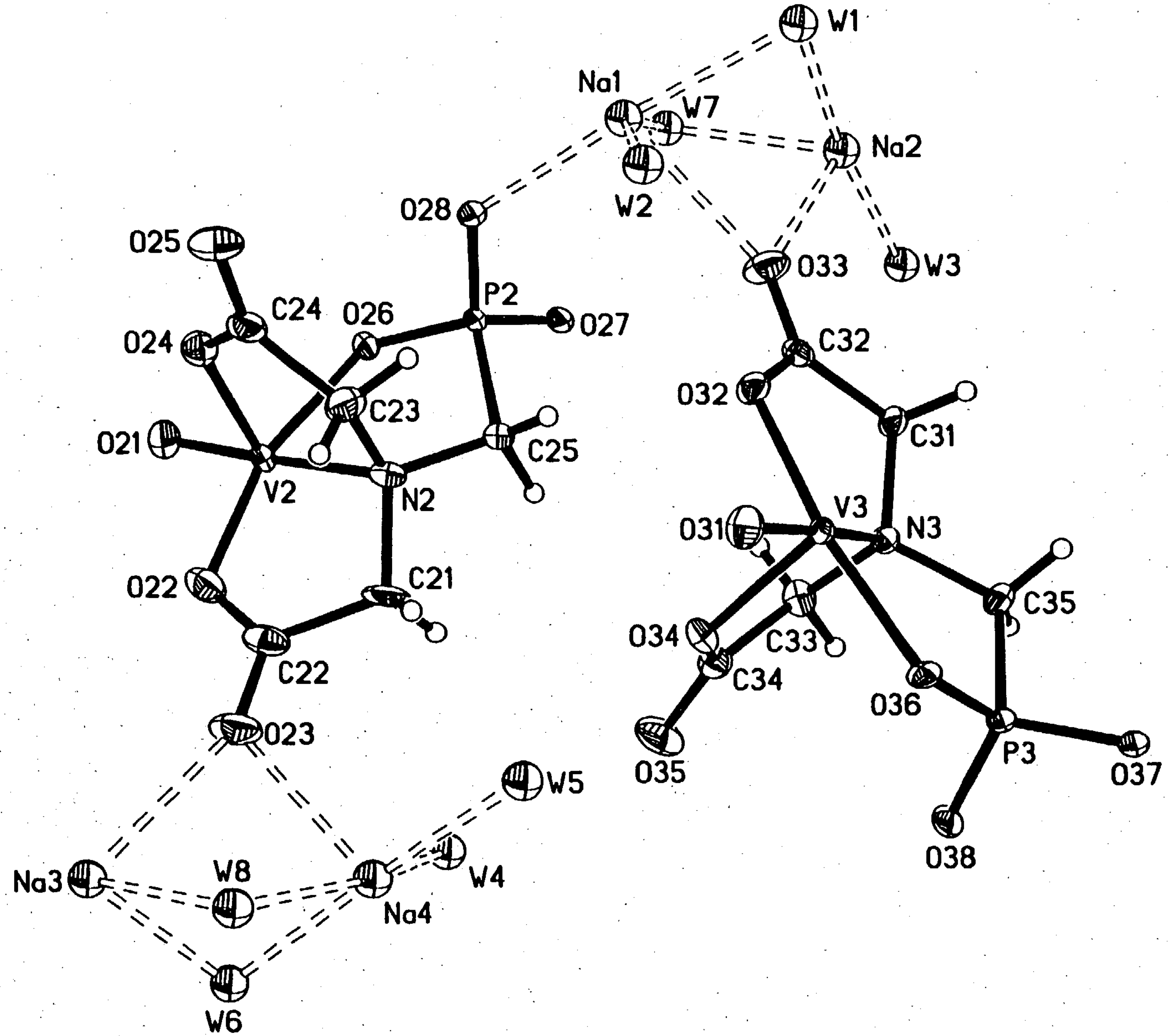
#7 -x+1,-y+1,-z+1   #8 -x+3/2,y+1/2,-z+1/2   #9 -x,-y+1,-z

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
V(1)	24(1)	8(1)	24(1)	0(1)	14(1)	3(1)
N(1)	16(2)	20(2)	27(2)	0(2)	10(2)	0(2)
P(1)	21(1)	9(1)	24(1)	0(1)	14(1)	3(1)
C(11)	14(2)	38(3)	45(3)	8(3)	11(2)	0(2)
C(12)	26(3)	37(3)	44(3)	20(3)	21(2)	10(2)
C(13)	23(2)	25(3)	25(2)	2(2)	6(2)	-1(2)
C(14)	21(2)	22(2)	30(3)	7(2)	11(2)	6(2)
C(15)	24(2)	14(2)	28(2)	-5(2)	11(2)	-4(2)
O(11)	56(3)	11(2)	33(2)	-5(2)	18(2)	-1(2)
O(12)	39(2)	26(2)	44(2)	14(2)	27(2)	16(2)
O(13)	28(2)	65(3)	77(4)	38(3)	32(2)	23(2)
O(14)	31(2)	18(2)	26(2)	4(1)	15(2)	1(1)
O(15)	32(2)	52(3)	25(2)	6(2)	12(2)	-7(2)
O(16)	21(2)	12(2)	25(2)	-2(1)	12(1)	0(1)
O(17)	26(2)	12(2)	29(2)	4(1)	16(1)	6(1)
O(18)	35(2)	17(2)	29(2)	3(1)	23(2)	4(1)
Na(1)	53(2)	18(1)	95(2)	3(1)	58(2)	4(1)
Na(2)	34(1)	39(1)	32(1)	-8(1)	16(1)	6(1)
W(1)	85(4)	21(2)	97(4)	4(2)	74(4)	2(2)
W(2)	33(2)	55(3)	37(2)	8(2)	15(2)	-17(2)
W(3)	43(2)	39(2)	40(2)	5(2)	20(2)	-8(2)
W(4)	105(6)	87(6)	93(5)	19(5)	35(5)	21(5)
W(5)	225(13)	184(11)	270(16)	170(11)	171(12)	151(10)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(11B)	8853(5)	4252(6)	2542(5)	38
H(11A)	8287(5)	4703(6)	1298(5)	38
H(13B)	6607(5)	3915(5)	3442(4)	30
H(13A)	7717(5)	3012(5)	3292(4)	30
H(15B)	6515(5)	5679(4)	1298(4)	25
H(15A)	6429(5)	5566(4)	2537(4)	25



W1
Na1
W7
Na2
W2
O28
O33
W3
O25
P2
C24
O26
O27
O24
C32
O32
C23
C31
O21
C25
V2
N2
V3
N3
O31
C21
C35
O22
O34
C33
C22
C34
O36
O23
P3
W5
O35
O37
W8
W4
Na3
Na4
O38
W6

Table 1. Crystal data and structure refinement for 2.

Identification code	dcccd15r
Empirical formula	$C_{10}H_{28}N_2Na_4O_{24}P_2V_2$
Formula weight	816.12
Temperature	164(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	*a* = 13.9822(2) Å alpha = 90°
	b = 11.1888(2) Å beta = 100.88°
	c = 18.6519(3) Å gamma = 90°
Volume, Z	2865.51(8) $Å^3$, 4
Density (calculated)	1.892 Mg/m^3
Absorption coefficient	0.926 mm^{-1}
F(000)	1656
Crystal size	0.38 x 0.24 x 0.08 mm
θ range for data collection	1.48 to 28.25°
Limiting indices	$-18 \le h \le 18$, $-13 \le k \le 14$, $-13 \le l \le 24$
Reflections collected	18164
Independent reflections	6790 (R_{int} = 0.0338)
Absorption correction	SADABS Tmax=0.83 Tmin=0.58
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6785 / 0 / 397
Goodness-of-fit on F^2	1.028
Final R indices [I>2σ(I)]	R1 = 0.0456, wR2 = 0.1100
R indices (all data)	R1 = 0.0670, wR2 = 0.1248
Largest diff. peak and hole	0.759 and -0.529 $eÅ^{-3}$

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

V(2)-O(21)	1.615(2)	V(2)-O(26)	1.990(2)
V(2)-O(27)#1	2.008(2)	V(2)-O(22)	2.024(2)
V(2)-O(24)	2.063(2)	V(2)-N(2)	2.362(2)
V(3)-O(31)	1.617(2)	V(3)-O(36)	1.987(2)
V(3)-O(37)#2	2.006(2)	V(3)-O(32)	2.041(2)
V(3)-O(34)	2.065(2)	V(3)-N(3)	2.361(2)
P(2)-O(28)	1.502(2)	P(2)-O(27)	1.554(2)
P(2)-O(26)	1.564(2)	P(2)-C(25)	1.837(3)
P(2)-Na(1)	3.4538(14)	P(3)-O(38)	1.504(2)
P(3)-O(37)	1.557(2)	P(3)-O(36)	1.559(2)
P(3)-C(35)	1.833(3)	P(3)-Na(3)#3	3.4536(14)
N(2)-C(21)	1.482(4)	N(2)-C(23)	1.488(4)
N(2)-C(25)	1.504(4)	N(3)-C(33)	1.481(4)
N(3)-C(31)	1.482(3)	N(3)-C(35)	1.500(3)
C(21)-C(22)	1.531(4)	C(22)-O(23)	1.243(4)
C(22)-O(22)	1.299(4)	C(23)-C(24)	1.530(4)
C(24)-O(25)	1.255(3)	C(24)-O(24)	1.280(3)
C(31)-C(32)	1.522(4)	C(32)-O(33)	1.240(4)
C(32)-O(32)	1.302(4)	C(33)-C(34)	1.523(4)
C(34)-O(35)	1.250(4)	C(34)-O(34)	1.277(4)
O(23)-Na(3)	2.462(2)	O(23)-Na(4)	2.504(3)
O(27)-V(2)#1	2.008(2)	O(28)-Na(1)	2.339(2)
O(28)-Na(2)#4	2.344(2)	O(33)-Na(2)	2.403(2)
O(33)-Na(1)	2.455(3)	O(37)-V(3)#2	2.006(2)
O(38)-Na(3)#3	2.332(2)	O(38)-Na(4)#5	2.381(2)
Na(1)-W(1)	2.374(3)	Na(1)-W(3)#4	2.432(3)
Na(1)-W(2)	2.474(3)	Na(1)-W(7)	2.496(3)
Na(1)-Na(2)	3.230(2)	Na(1)-Na(2)#4	3.335(2)
Na(2)-W(7)	2.305(3)	Na(2)-O(28)#6	2.344(2)
Na(2)-W(3)	2.399(3)	Na(2)-W(1)	2.408(3)
Na(2)-Na(1)#6	3.335(2)	Na(3)-W(6)	2.303(2)
Na(3)-O(38)#7	2.332(2)	Na(3)-W(2)#8	2.463(3)
Na(3)-W(5)#9	2.502(2)	Na(3)-W(8)	2.581(3)
Na(3)-Na(4)	3.261(2)	Na(3)-P(3)#7	3.4538(14)
Na(3)-Na(4)#9	3.477(2)	Na(4)-W(8)	2.375(3)
Na(4)-O(38)#9	2.381(2)	Na(4)-W(5)	2.403(2)
Na(4)-W(6)	2.431(3)	Na(4)-W(4)	2.439(3)
Na(4)-Na(3)#5	3.477(2)	W(2)-Na(3)#10	2.463(3)
W(3)-Na(1)#6	2.432(3)	W(5)-Na(3)#5	2.502(2)

O(21)-V(2)-O(26)	105.60(10)	O(21)-V(2)-O(27)#1	102.01(10)
O(26)-V(2)-O(27)#1	88.72(8)	O(21)-V(2)-O(22)	99.93(10)
O(26)-V(2)-O(22)	154.35(9)	O(27)#1-V(2)-O(22)	88.46(8)
O(21)-V(2)-O(24)	92.25(10)	O(26)-V(2)-O(24)	86.38(8)
O(27)#1-V(2)-O(24)	165.70(8)	O(22)-V(2)-O(24)	90.16(8)
O(21)-V(2)-N(2)	167.54(10)	O(26)-V(2)-N(2)	79.21(8)
O(27)#1-V(2)-N(2)	89.46(8)	O(22)-V(2)-N(2)	75.27(8)
O(24)-V(2)-N(2)	76.43(8)	O(31)-V(3)-O(36)	105.45(10)
O(31)-V(3)-O(37)#2	101.08(10)	O(36)-V(3)-O(37)#2	88.97(8)
O(31)-V(3)-O(32)	100.18(10)	O(36)-V(3)-O(32)	154.29(8)
O(37)#2-V(3)-O(32)	88.12(8)	O(31)-V(3)-O(34)	93.84(10)
O(36)-V(3)-O(34)	85.43(8)	O(37)#2-V(3)-O(34)	164.99(9)
O(32)-V(3)-O(34)	90.90(8)	O(31)-V(3)-N(3)	168.17(10)
O(36)-V(3)-N(3)	79.89(8)	O(37)#2-V(3)-N(3)	89.44(8)

O(32)-V(3)-N(3)	74.54(8)	O(34)-V(3)-N(3)	75.88(8)
O(28)-P(2)-O(27)	112.30(11)	O(28)-P(2)-O(26)	112.16(11)
O(27)-P(2)-O(26)	109.11(11)	O(28)-P(2)-C(25)	110.29(13)
O(27)-P(2)-C(25)	109.79(12)	O(26)-P(2)-C(25)	102.76(12)
O(28)-P(2)-Na(1)	32.88(8)	O(27)-P(2)-Na(1)	88.98(8)
O(26)-P(2)-Na(1)	144.46(8)	C(25)-P(2)-Na(1)	99.11(10)
O(38)-P(3)-O(37)	112.38(11)	O(38)-P(3)-O(36)	112.36(12)
O(37)-P(3)-O(36)	109.49(11)	O(38)-P(3)-C(35)	109.87(13)
O(37)-P(3)-C(35)	109.07(12)	O(36)-P(3)-C(35)	103.24(12)
O(38)-P(3)-Na(3)#3	32.58(8)	O(37)-P(3)-Na(3)#3	93.49(8)
O(36)-P(3)-Na(3)#3	144.90(8)	C(35)-P(3)-Na(3)#3	93.30(10)
C(21)-N(2)-C(23)	111.5(2)	C(21)-N(2)-C(25)	112.9(2)
C(23)-N(2)-C(25)	111.4(2)	C(21)-N(2)-V(2)	103.4(2)
C(23)-N(2)-V(2)	108.0(2)	C(25)-N(2)-V(2)	109.3(2)
C(33)-N(3)-C(31)	111.2(2)	C(33)-N(3)-C(35)	111.9(2)
C(31)-N(3)-C(35)	112.5(2)	C(33)-N(3)-V(3)	108.0(2)
C(31)-N(3)-V(3)	104.1(2)	C(35)-N(3)-V(3)	108.8(2)
N(2)-C(21)-C(22)	110.5(2)	O(23)-C(22)-O(22)	124.0(3)
O(23)-C(22)-C(21)	119.6(3)	O(22)-C(22)-C(21)	116.4(2)
N(2)-C(23)-C(24)	113.0(2)	O(25)-C(24)-O(24)	123.6(3)
O(25)-C(24)-C(23)	118.2(3)	O(24)-C(24)-C(23)	118.2(2)
N(2)-C(25)-P(2)	108.5(2)	N(3)-C(31)-C(32)	109.9(2)
O(33)-C(32)-O(32)	123.8(3)	O(33)-C(32)-C(31)	119.2(3)
O(32)-C(32)-C(31)	116.9(2)	N(3)-C(33)-C(34)	112.4(2)
O(35)-C(34)-O(34)	123.4(3)	O(35)-C(34)-C(33)	119.0(3)
O(34)-C(34)-C(33)	117.6(3)	N(3)-C(35)-P(3)	108.9(2)
C(22)-O(22)-V(2)	121.6(2)	C(22)-O(23)-Na(3)	154.8(2)
C(22)-O(23)-Na(4)	122.9(2)	Na(3)-O(23)-Na(4)	82.06(7)
C(24)-O(24)-V(2)	122.7(2)	P(2)-O(26)-V(2)	127.05(11)
P(2)-O(27)-V(2)#1	138.16(12)	P(2)-O(28)-Na(1)	126.71(12)
P(2)-O(28)-Na(2)#4	129.30(12)	Na(1)-O(28)-Na(2)#4	90.82(8)
C(32)-O(32)-V(3)	121.2(2)	C(32)-O(33)-Na(2)	138.7(2)
C(32)-O(33)-Na(1)	137.0(2)	Na(2)-O(33)-Na(1)	83.32(8)
C(34)-O(34)-V(3)	122.7(2)	P(3)-O(36)-V(3)	126.24(12)
P(3)-O(37)-V(3)#2	137.84(12)	P(3)-O(38)-Na(3)#3	127.10(12)
P(3)-O(38)-Na(4)#5	125.36(12)	Na(3)#3-O(38)-Na(4)#5	95.10(8)
O(28)-Na(1)-W(1)	161.08(9)	O(28)-Na(1)-W(3)#4	89.86(9)
W(1)-Na(1)-W(3)#4	91.20(9)	O(28)-Na(1)-O(33)	101.23(9)
W(1)-Na(1)-O(33)	74.09(9)	W(3)#4-Na(1)-O(33)	162.87(10)
O(28)-Na(1)-W(2)	106.56(9)	W(1)-Na(1)-W(2)	90.91(9)
W(3)#4-Na(1)-W(2)	109.25(10)	O(33)-Na(1)-W(2)	80.27(9)
O(28)-Na(1)-W(7)	79.44(8)	W(1)-Na(1)-W(7)	81.67(8)
W(3)#4-Na(1)-W(7)	90.28(10)	O(33)-Na(1)-W(7)	79.13(9)
W(2)-Na(1)-W(7)	159.31(10)	O(28)-Na(1)-Na(2)	115.34(7)
W(1)-Na(1)-Na(2)	47.95(6)	W(3)#4-Na(1)-Na(2)	115.71(8)
O(33)-Na(1)-Na(2)	47.65(6)	W(2)-Na(1)-Na(2)	116.74(7)
W(7)-Na(1)-Na(2)	45.27(6)	O(28)-Na(1)-Na(2)#4	44.66(6)
W(1)-Na(1)-Na(2)#4	130.48(8)	W(3)#4-Na(1)-Na(2)#4	45.93(7)
O(33)-Na(1)-Na(2)#4	140.91(8)	W(2)-Na(1)-Na(2)#4	122.16(8)
W(7)-Na(1)-Na(2)#4	76.27(7)	Na(2)-Na(1)-Na(2)#4	121.02(4)
O(28)-Na(1)-P(2)	20.41(5)	W(1)-Na(1)-P(2)	145.95(7)
W(3)#4-Na(1)-P(2)	107.86(7)	O(33)-Na(1)-P(2)	81.45(7)
W(2)-Na(1)-P(2)	108.10(7)	W(7)-Na(1)-P(2)	70.60(6)
Na(2)-Na(1)-P(2)	98.01(4)	Na(2)#4-Na(1)-P(2)	61.94(3)
W(7)-Na(2)-O(28)#6	98.75(9)	W(7)-Na(2)-W(3)	101.94(10)
O(28)#6-Na(2)-W(3)	90.54(9)	W(7)-Na(2)-O(33)	84.07(9)
O(28)#6-Na(2)-O(33)	161.46(10)	W(3)-Na(2)-O(33)	106.89(10)
W(7)-Na(2)-W(1)	85.03(9)	O(28)#6-Na(2)-W(1)	87.49(8)

W(3)-Na(2)-W(1)	172.98(11)	O(33)-Na(2)-W(1)	74.45(8)
W(7)-Na(2)-Na(1)	50.27(7)	O(28)#6-Na(2)-Na(1)	119.96(7)
W(3)-Na(2)-Na(1)	138.87(8)	O(33)-Na(2)-Na(1)	49.03(6)
W(1)-Na(2)-Na(1)	47.08(6)	W(7)-Na(2)-Na(1)#6	111.26(7)
O(28)#6-Na(2)-Na(1)#6	44.52(6)	W(3)-Na(2)-Na(1)#6	46.76(7)
O(33)-Na(2)-Na(1)#6	150.58(8)	W(1)-Na(2)-Na(1)#6	129.93(7)
Na(1)-Na(2)-Na(1)#6	158.18(5)	W(6)-Na(3)-O(38)#7	160.15(9)
W(6)-Na(3)-W(2)#8	113.14(9)	O(38)#7-Na(3)-W(2)#8	85.14(8)
W(6)-Na(3)-O(23)	79.62(8)	O(38)#7-Na(3)-O(23)	100.48(8)
W(2)#8-Na(3)-O(23)	114.17(9)	W(6)-Na(3)-W(5)#9	88.10(8)
O(38)#7-Na(3)-W(5)#9	86.69(8)	W(2)#8-Na(3)-W(5)#9	82.57(8)
O(23)-Na(3)-W(5)#9	162.11(9)	W(6)-Na(3)-W(8)	80.57(8)
O(38)#7-Na(3)-W(8)	79.93(8)	W(2)#8-Na(3)-W(8)	161.34(9)
O(23)-Na(3)-W(8)	79.79(8)	W(5)#9-Na(3)-W(8)	85.43(8)
W(6)-Na(3)-Na(4)	48.13(6)	O(38)#7-Na(3)-Na(4)	117.38(7)
W(2)#8-Na(3)-Na(4)	152.45(8)	O(23)-Na(3)-Na(4)	49.52(6)
W(5)#9-Na(3)-Na(4)	112.63(7)	W(8)-Na(3)-Na(4)	46.19(6)
W(6)-Na(3)-P(3)#7	147.10(7)	O(38)#7-Na(3)-P(3)#7	20.32(5)
W(2)#8-Na(3)-P(3)#7	99.08(7)	O(23)-Na(3)-P(3)#7	81.30(6)
W(5)#9-Na(3)-P(3)#7	103.07(6)	W(8)-Na(3)-P(3)#7	69.80(6)
Na(4)-Na(3)-P(3)#7	99.46(4)	W(6)-Na(3)-Na(4)#9	128.58(7)
O(38)#7-Na(3)-Na(4)#9	42.99(6)	W(2)#8-Na(3)-Na(4)#9	82.34(7)
O(23)-Na(3)-Na(4)#9	140.52(7)	W(5)#9-Na(3)-Na(4)#9	43.71(6)
W(8)-Na(3)-Na(4)#9	79.11(6)	Na(4)-Na(3)-Na(4)#9	124.74(4)
P(3)#7-Na(3)-Na(4)#9	60.18(3)	W(8)-Na(4)-O(38)#9	88.39(8)
W(8)-Na(4)-W(5)	93.16(9)	O(38)#9-Na(4)-W(5)	87.91(8)
W(8)-Na(4)-W(6)	82.38(8)	O(38)#9-Na(4)-W(6)	88.06(8)
W(5)-Na(4)-W(6)	174.07(9)	W(8)-Na(4)-W(4)	162.20(10)
O(38)#9-Na(4)-W(4)	100.38(10)	W(5)-Na(4)-W(4)	102.53(9)
W(6)-Na(4)-W(4)	82.48(9)	W(8)-Na(4)-O(23)	83.05(8)
O(38)#9-Na(4)-O(23)	163.13(9)	W(5)-Na(4)-O(23)	107.01(9)
W(6)-Na(4)-O(23)	76.43(8)	W(4)-Na(4)-O(23)	84.36(10)
W(8)-Na(4)-Na(3)	51.65(6)	O(38)#9-Na(4)-Na(3)	115.29(7)
W(5)-Na(4)-Na(3)	134.08(7)	W(6)-Na(4)-Na(3)	44.86(6)
W(4)-Na(4)-Na(3)	110.60(8)	O(23)-Na(4)-Na(3)	48.41(6)
W(8)-Na(4)-Na(3)#5	91.76(7)	O(38)#9-Na(4)-Na(3)#5	41.90(6)
W(5)-Na(4)-Na(3)#5	46.02(6)	W(6)-Na(4)-Na(3)#5	129.89(7)
W(4)-Na(4)-Na(3)#5	105.14(8)	O(23)-Na(4)-Na(3)#5	152.40(7)
Na(3)-Na(4)-Na(3)#5	141.33(4)	Na(1)-W(1)-Na(2)	84.97(8)
Na(3)#10-W(2)-Na(1)	131.07(11)	Na(2)-W(3)-Na(1)#6	87.31(9)
Na(4)-W(5)-Na(3)#5	90.27(8)	Na(3)-W(6)-Na(4)	87.01(8)
Na(2)-W(7)-Na(1)	84.46(8)	Na(4)-W(8)-Na(3)	82.17(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z   #2 -x+1,-y+1,-z   #3 x,y-1,z   #4 -x,y+1/2,-z-1/2

#5 -x+1,y-1/2,-z+1/2   #6 -x,y-1/2,-z-1/2   #7 x,y+1,z

#8 x,-y+5/2,z+1/2   #9 -x+1,y+1/2,-z+1/2   #10 x,-y+5/2,z-1/2

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
V(2)	14(1)	15(1)	12(1)	-1(1)	2(1)	0(1)
V(3)	14(1)	14(1)	11(1)	1(1)	1(1)	-1(1)
P(2)	15(1)	15(1)	10(1)	-1(1)	2(1)	-1(1)
P(3)	15(1)	14(1)	9(1)	1(1)	1(1)	1(1)
N(2)	13(1)	18(1)	11(1)	0(1)	0(1)	-1(1)
N(3)	13(1)	14(1)	11(1)	0(1)	1(1)	0(1)
C(21)	17(1)	24(2)	15(1)	-1(1)	-3(1)	0(1)
C(22)	21(2)	23(2)	12(1)	2(1)	1(1)	-6(1)
C(23)	15(1)	19(1)	20(2)	1(1)	6(1)	-2(1)
C(24)	18(1)	18(1)	13(1)	-1(1)	3(1)	-5(1)
C(25)	15(1)	16(1)	15(1)	0(1)	2(1)	-1(1)
C(31)	17(1)	18(1)	13(1)	-2(1)	-2(1)	-3(1)
C(32)	19(1)	21(2)	12(1)	-1(1)	2(1)	3(1)
C(33)	16(1)	22(2)	16(1)	-4(1)	6(1)	0(1)
C(34)	16(1)	22(2)	16(1)	-3(1)	0(1)	1(1)
C(35)	15(1)	14(1)	16(1)	2(1)	-1(1)	-1(1)
O(21)	20(1)	23(1)	23(1)	-3(1)	5(1)	3(1)
O(22)	19(1)	20(1)	17(1)	-4(1)	1(1)	-4(1)
O(23)	26(1)	30(1)	17(1)	0(1)	-7(1)	-7(1)
O(24)	19(1)	19(1)	17(1)	2(1)	4(1)	-1(1)
O(25)	23(1)	28(1)	16(1)	5(1)	6(1)	-2(1)
O(26)	15(1)	19(1)	11(1)	-1(1)	1(1)	0(1)
O(27)	20(1)	18(1)	11(1)	0(1)	1(1)	-4(1)
O(28)	22(1)	19(1)	12(1)	1(1)	4(1)	-1(1)
O(31)	21(1)	22(1)	23(1)	4(1)	4(1)	-4(1)
O(32)	18(1)	18(1)	16(1)	3(1)	0(1)	1(1)
O(33)	24(1)	33(1)	19(1)	5(1)	-8(1)	-2(1)
O(34)	19(1)	19(1)	19(1)	-5(1)	4(1)	-2(1)
O(35)	22(1)	42(1)	21(1)	-15(1)	7(1)	-2(1)
O(36)	16(1)	17(1)	12(1)	3(1)	1(1)	0(1)
O(37)	19(1)	17(1)	11(1)	0(1)	1(1)	4(1)
O(38)	23(1)	18(1)	11(1)	0(1)	3(1)	0(1)
Na(1)	22(1)	23(1)	17(1)	-1(1)	3(1)	1(1)
Na(2)	28(1)	28(1)	19(1)	-1(1)	1(1)	-6(1)
Na(3)	22(1)	22(1)	17(1)	1(1)	4(1)	-1(1)
Na(4)	26(1)	23(1)	16(1)	-1(1)	1(1)	2(1)
W(1)	26(1)	38(1)	20(1)	-9(1)	6(1)	-9(1)
W(2)	25(1)	29(1)	33(1)	0(1)	8(1)	-3(1)
W(3)	72(2)	30(1)	20(1)	-3(1)	9(1)	-16(1)
W(4)	56(2)	39(2)	45(2)	-8(1)	13(1)	-11(1)
W(5)	28(1)	21(1)	17(1)	0(1)	2(1)	-1(1)
W(6)	22(1)	26(1)	17(1)	4(1)	3(1)	2(1)
W(7)	23(1)	37(1)	21(1)	-8(1)	1(1)	0(1)
W(8)	31(1)	25(1)	18(1)	6(1)	4(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(21A)	3166(2)	11007(3)	712(2)	23
H(21B)	2266(2)	10490(3)	1035(2)	23
H(23A)	2515(2)	11198(3)	-892(2)	21
H(23B)	2986(2)	12114(3)	-266(2)	21
H(25A)	1458(2)	9406(3)	153(2)	18
H(25B)	2058(2)	9536(3)	-497(2)	18
H(31A)	1773(2)	5675(3)	-569(2)	20
H(31B)	2662(2)	5205(3)	-925(2)	20
H(33A)	2495(2)	6084(3)	973(2)	21
H(33B)	1994(2)	6969(3)	338(2)	21
H(35A)	3603(2)	4292(3)	-38(2)	19
H(35B)	3076(2)	4443(3)	649(2)	19