

## The Crystal and Molecular Structure of Sodium $\mu$ -Triethylenetetraaminehexaacetatodi-[oxo-vanadium(IV)] Decahydrate, $\text{Na}_2[(\text{VO})_2\text{TTHA}] \cdot 10\text{H}_2\text{O}$

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$\text{Na}_2[(\text{VO})_2\text{TTHA}] \cdot 10\text{H}_2\text{O}$  is triclinic, space group  $P\bar{1}$ , with  $a=10.003(5)$ ,  $b=14.905(8)$ ,  $c=6.630(4)$  Å,  $\alpha=77.55(8)$ ,  $\beta=108.65(11)$ ,  $\gamma=111.19(11)^\circ$ ,  $D_m=1.62(2)$ ,  $D_c=1.62$  g cm $^{-3}$  for  $Z=1$ . With 2286 statistically significant, counter-measured reflexions, the structure was determined by direct and Fourier methods and refined to an  $R$  of 0.056. The discrete binuclear units,  $[(\text{VO})_2\text{TTHA}]^{2-}$ , are required crystallographically to be centrosymmetric. The coordination distances are: V–O(oxo), 1.605(8); V–O, 1.986(4), 1.986(4), 2.006(5); V–N, 2.163(5), 2.294(7) Å.

### Introduction

A recent study of vanadyl complexes with the aminopolycarboxylic acids, ethylenediaminetetraacetic acid (EDTA), 3,6-dioxaoctane-1,8-diamine- $N,N,N',N'$ -tetraacetic acid (EGTA), diethylenetriaminepentaacetic acid (DTPA) and triethylenetetraaminehexaacetic acid (TTHA) indicated that at certain mole ratios and  $p\text{H}$ , monomeric, dimeric and dinuclear complexes are formed (Smith, Boas & Pilbrow, 1974).

Potentiometric  $p\text{H}$  titrations show that in solutions containing vanadyl ion and TTHA in a 2:1 mole ratio only one major vanadyl complex is formed in the  $p\text{H}$  range *ca* 4 to 10. The X-band e.s.r. spectrum of an aqueous solution of this composition, at room temperature, consisted only of a 15 line signal in the  $g=2$  region which did not vary in the  $p\text{H}$  range 2.1 to 10.6. This observation and the positions of the peaks in the spectra were attributed to the formation of a binuclear chelate, where the vanadyl ions are coupled by exchange interactions, but no suitable explanation for the coupling mechanism could be offered.

The present analysis was undertaken in the hope that the solid-state structure of the binuclear chelate would render assistance in the interpretation of the exchange coupling mechanism.

### Experimental

Royal-blue rectangular crystals elongated along [001] were grown from a saturated aqueous solution in a sealed glass tube which was cooled from *ca* 90°C to room temperature over a three day period. The original compound was obtained from an aqueous solution containing 0.1 mole vanadyl sulphate and 0.05 mole  $\text{H}_6\text{TTHA}$  at *ca*  $p\text{H}$  7.0, the  $p\text{H}$  being initially adjusted by the addition of 0.1  $M$  NaOH. The crystals turn to a light blue powder on standing through loss of water of crystallization.

### Crystal data

$\text{C}_{18}\text{H}_{44}\text{O}_{24}\text{N}_4\text{V}_2\text{Na}_2$ ,  $M=848.54$ , triclinic,  $a=10.003(5)$ ,  $b=14.905(8)$ ,  $c=6.630(4)$  Å,  $\alpha=77.55(8)$ ,  $\beta=108.65(11)$ ,  $\gamma=111.19(11)^\circ$ ,  $U=867.7$  Å $^3$ ,  $D_m=1.62(2)$  g cm $^{-3}$  (by flotation in carbon tetrachloride–1,1,2,2-tetrabromoethane),  $Z=1$ ,  $D_c=1.62$  g cm $^{-3}$ ,  $F(000)=440$ ,  $\mu=7.0$  cm $^{-1}$  for Mo  $K\alpha$  radiation ( $\lambda=0.7107$  Å). Space group  $P1$  or  $P\bar{1}$ , ( $P\bar{1}$  from successful refinement). Cell parameters were obtained with a Philips PW 1100 diffractometer.

### Intensity measurements

Intensities were collected from a single crystal,  $0.19 \times 0.11 \times 0.12$  mm, sealed inside a 0.3 mm Lindemann tube with a drop of mother liquor. 4188 unique reflexions were collected out to  $2\theta$  (Mo  $K\alpha$ ) = 56.0°, with the diffractometer and graphite-monochromated Mo  $K\alpha$  radiation. 2286 were considered to be significantly above background [ $I \geq 3\sigma(I)$ ], and were used in the subsequent calculations. Three standard reflexions monitored at two-hourly intervals showed a significant decrease in intensity, for which  $I$  was corrected.

The data were collected by the  $\omega$ -scan technique with a symmetric scan range of  $\pm 0.45^\circ$  in  $\theta$ , with an allowance for dispersion, from the calculated Bragg scattering angle, at a scan rate of 0.06° s $^{-1}$ . No reflexion was sufficiently intense to require the insertion of an attenuation filter.

Data were processed with a program written for the diffractometer (Hornstra & Stubbe, 1972). The background-corrected intensities were assigned standard deviations according to:

$$\sigma(I) = [\text{CT} + (t_c/t_b)^2(B_1 + B_2) + (pI)^2]^{1/2}$$

where CT is the total integrated peak count obtained in a scan time  $t_c$ ;  $B_1$  and  $B_2$  are background counts each obtained in time  $\frac{1}{2}t_b$ ; and  $I = \text{CT} - (t_c/t_b)(B_1 + B_2)$ ;  $p$  was 0.04 to allow for other error sources. Values

of  $I$  and  $\sigma(I)$  were then corrected for Lorentz and polarization effects, but not for extinction or absorption.

#### Structure determination and refinement

The 2286 significant reflexions were placed on an absolute scale by Wilson's method and converted to  $E$  values (Shiono, 1964). Several sets of phases were generated from the 390  $E$  values greater than 1.62 with *MULTAN* (Germain, Main & Woolfson, 1970). An  $E$  map, computed from the set which produced the highest internal consistency, revealed the location of all non-hydrogen atoms in the anion. A structure-factor calculation based on these atomic positions with an isotropic thermal parameter of  $3.0 \text{ \AA}^2$  gave  $R_1$  and  $R_2$ , 0.350 and 0.398 respectively. ( $R_1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|}$  and  $R_2 = \frac{[\sum w(|F_o| - |F_c|)^2]}{[\sum w|F_o|^2]}^{1/2}$ .)

In the least-squares calculations, the function minimized was  $\sum w(|F_o| - |F_c|)^2$ . A difference synthesis revealed six additional peaks, one being a Na atom, the others O atoms of water molecules. After several cycles of full-matrix least-squares refinement the positional and isotropic thermal parameters converged to give  $R_1$  0.098 and  $R_2$  0.111. Several further cycles of block-diagonal least-squares refinement, with anisotropic thermal parameters, converged to give  $R_1$  0.067 and  $R_2$  0.078.

A difference synthesis clearly revealed all the H atoms, except those of the water molecules, which were included in the calculations at idealized positions, (C-H 0.95 Å; Churchill, 1973), Table 1, with isotropic thermal parameters of  $5.0 \text{ \AA}^2$ . Refinement was con-

tinued with fixed H parameters and was considered complete when no parameter shift was greater than  $0.1\sigma$ . The final residuals for observed reflexions were  $R_1$  0.056,  $R_2$  0.063; for all reflexions  $R_1$  0.126,  $R_2$  0.073. The estimated standard deviation of an observation of unit weight was 1.246.

Table 1. Idealized hydrogen atom positions ( $\times 10^3$ )

	$x$	$y$	$z$
H(C1)A	-53	488	681
H(C1)B	-103	408	533
H(C2)A	70	345	492
H(C2)B	218	430	518
H(C3)A	265	281	641
H(C3)B	328	346	826
H(C4)A	45	167	591
H(C4)B	15	100	798
H(C6)A	242	136	1013
H(C6)B	320	235	1107
H(C8)A	300	534	753
H(C8)B	191	554	846

A final difference synthesis had no major characteristics greater than  $0.3 \text{ e \AA}^{-3}$ .

Scattering factors used were those of Cromer & Waber (1965) for V, O, C, N and Ibers (1962) for H. Other major programs used during refinement were modified versions of the full-matrix least-squares program *ORFLS* (Busing, Martin & Levy, 1962) the block-diagonal least-squares program of Shiono (1968) and the Fourier summation program of White (1965). All figures were drawn with Johnson's (1965) *ORTEP*. All major calculations were performed on the Monash University CDC 3200 computer.

Table 2. Final positional parameters ( $\times 10^4$ ) and anisotropic thermal parameters ( $\times 10^3$ ) of non-hydrogen atoms

	$x$	$y$	$z$	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
V*	351 (1)	3175 (1)	9830 (2)	256 (6)	259 (6)	196 (5)	121 (4)	60 (4)	-21 (4)
Na	-3537 (3)	-296 (2)	4660 (5)	39 (2)	34 (2)	40 (2)	13 (1)	9 (1)	-4 (1)
O(V)	-602 (6)	3630 (4)	10612 (8)	53 (3)	52 (3)	41 (3)	26 (3)	20 (3)	-9 (3)
O(1)	-2349 (6)	1322 (4)	5422 (9)	38 (3)	48 (3)	60 (4)	4 (3)	-4 (3)	-25 (3)
O(2)	-1337 (5)	2444 (3)	7630 (8)	24 (2)	34 (3)	43 (3)	8 (2)	4 (2)	-13 (2)
O(3)	1511 (7)	879 (4)	13535 (9)	63 (4)	62 (4)	54 (4)	40 (3)	28 (3)	26 (3)
O(4)	416 (6)	1995 (4)	11944 (8)	44 (3)	44 (3)	35 (3)	25 (3)	17 (2)	9 (2)
O(5)	4248 (6)	5233 (5)	11610 (9)	43 (3)	70 (4)	51 (3)	-2 (3)	-3 (3)	-30 (3)
O(6)	2427 (5)	3835 (4)	11399 (7)	37 (3)	41 (3)	27 (3)	9 (2)	1 (2)	-4 (2)
O(7)	-4526 (6)	-383 (4)	7666 (8)	41 (3)	48 (3)	41 (3)	13 (3)	11 (3)	-4 (3)
O(8)	-2296 (8)	292 (5)	1712 (11)	82 (5)	95 (6)	70 (5)	-30 (4)	46 (4)	-46 (4)
O(9)	-5234 (6)	-1866 (4)	4123 (11)	38 (3)	47 (3)	86 (5)	8 (3)	14 (3)	-13 (3)
O(10)	-3807 (9)	2050 (6)	308 (12)	107 (6)	90 (6)	74 (5)	-18 (5)	31 (5)	3 (5)
O(11)	-4653 (7)	3774 (4)	4949 (9)	74 (4)	55 (4)	52 (4)	31 (3)	23 (3)	4 (3)
N(1)	1048 (6)	4249 (4)	7285 (8)	28 (3)	26 (3)	21 (3)	11 (3)	4 (2)	-2 (2)
N(2)	1423 (6)	2369 (4)	8553 (8)	24 (3)	28 (3)	25 (3)	12 (2)	4 (2)	-3 (2)
C(1)	-206 (8)	4613 (5)	5928 (10)	31 (4)	31 (4)	26 (4)	15 (3)	9 (3)	4 (3)
C(2)	1552 (8)	3799 (5)	5947 (11)	35 (4)	31 (4)	25 (4)	12 (3)	10 (3)	-3 (3)
C(3)	2381 (7)	3112 (5)	7303 (11)	27 (3)	25 (3)	31 (4)	11 (3)	11 (3)	2 (3)
C(4)	212 (7)	1637 (5)	7226 (12)	25 (4)	29 (4)	38 (4)	6 (3)	6 (3)	-9 (3)
C(5)	-1272 (7)	1803 (5)	6697 (11)	29 (4)	27 (4)	30 (4)	5 (3)	6 (3)	-2 (3)
C(6)	2251 (8)	1896 (5)	10489 (11)	30 (4)	39 (4)	35 (4)	20 (3)	11 (3)	5 (2)
C(7)	1342 (8)	1546 (5)	12129 (12)	27 (4)	38 (4)	36 (4)	13 (3)	6 (3)	1 (3)
C(8)	2297 (8)	5051 (5)	8377 (11)	32 (4)	23 (4)	36 (4)	2 (3)	7 (3)	-8 (3)
C(9)	3073 (8)	4695 (6)	10619 (11)	28 (4)	46 (5)	31 (4)	10 (3)	3 (3)	-17 (3)

\* For V thermal parameters are  $\times 10^4$ .

Final positional and vibrational parameters are listed in Table 2.\* The atom labelling is shown in Fig. 1.

### Results and discussion

Table 3 gives the intramolecular distances and angles in the vanadyl TTHA ion; a stereoscopic view of the binuclear complex is shown in Fig. 2, the mid-point of C(1)–C(1') being a required centre of inversion.

The V atom is octahedrally coordinated to the oxo ligand and three O and two N atoms of the TTHA ligand, the complex utilizing all the coordination sites of TTHA which is fully ionized. The coordination octahedron of the V atom is distorted as evidenced by the 12 octahedral edge lengths which vary from 2.623 to 2.967 Å. Moreover, an examination of Fig. 2, together with the listing in Table 4 of the atomic displacements from the three principal coordination planes of the octahedron, shows that the V atom is displaced 0.39 Å from the octahedral centre towards the oxo ligand.

\* A list of observed and calculated structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31132 (19 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

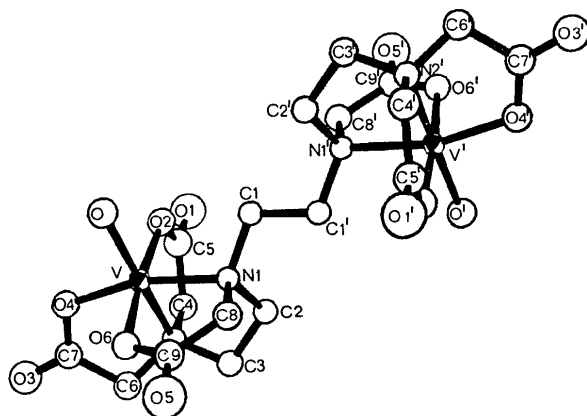


Fig. 1. Projection of the molecule indicating the numbering system used for the TTHA ligand. Primed labels represent atoms related by centre of inversion.

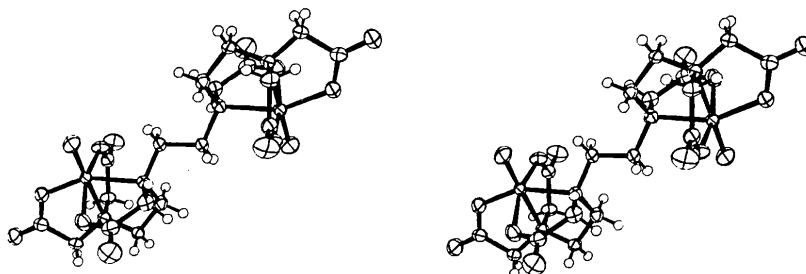


Fig. 2. Stereoscopic diagram of  $[(VO)_2TTHA]^{2-}$ , showing 50% probability ellipsoids, except those for H atoms which have been reduced for clarity.

Table 3. Bond lengths (Å) and angles (°) with estimated standard deviations in parentheses

V—O(V)	1.605 (8)	V—O(6)	1.986 (4)
V—O(2)	1.986 (4)	V—N(1)	2.163 (5)
V—O(4)	2.006 (5)	V—N(2)	2.294 (7)
C(1)–C(1')	1.543 (11)	N(2)–C(6)	1.477 (8)
C(1)–N(1)	1.496 (9)	C(6)–C(7)	1.525 (12)
N(1)–C(2)	1.508 (11)	C(7)–O(4)	1.288 (11)
N(2)–C(3)	1.476 (8)	C(7)–O(3)	1.228 (9)
C(2)–C(3)	1.511 (10)	N(1)–C(8)	1.493 (8)
N(2)–C(4)	1.486 (8)	C(8)–C(9)	1.521 (9)
C(4)–C(5)	1.511 (11)	C(9)–O(6)	1.287 (8)
C(5)–O(2)	1.276 (11)	C(9)–O(5)	1.228 (8)
C(5)–O(1)	1.228(8)		

#### V–V distances (Å)

	Intramolecular	7.482	
	Intermolecular	5.791	
N(1)–V—O(4)	153.5 (2)	N(2)–C(3)–C(2)	108.9 (6)
N(2)–V—O(V)	172.5 (3)	V—N(1)–C(2)	109.0 (4)
O(2)–V—O(6)	159.7 (2)	V—N(2)–C(3)	106.1 (4)
C(1')–C(1)–N(1)	113.4 (7)	N(1)–V—N(2)	80.2 (2)
N(1)–C(2)–C(3)	111.9 (6)		
V—O(2)–C(5)	124.0 (5)	V—O(4)–C(7)	121.4 (5)
V—N(2)–C(4)	108.0 (4)	V—N(2)–C(6)	104.7 (4)
N(2)–C(4)–C(5)	112.1 (6)	N(2)–C(6)–C(7)	108.4 (6)
O(2)–C(5)–C(4)	117.2 (6)	O(4)–C(7)–C(6)	116.0 (7)
N(2)–V—O(2)	76.8 (2)	N(2)–V—O(4)	94.0 (2)
V—O(6)–C(9)	117.5 (5)	O(6)–C(9)–C(8)	117.1 (7)
V—N(1)–C(8)	105.6 (4)	N(1)–V—O(6)	80.5 (2)
N(1)–C(8)–C(9)	111.8 (6)		

The V to oxo O length of 1.605 (8) Å is typical of the vanadyl linkage and falls in the middle of the range of values, 1.57–1.62 Å, reported (Mathew, Carty & Palenik, 1970; Scheidt, 1973). As is to be expected, owing to the *trans* effect of the oxo ligand (Scheidt, 1973), the V–N(2) linkage of 2.294 (7) Å is significantly longer than the *cis* V–N(1) linkage, 2.163 (5) Å. V–N(2) is slightly shorter than that found in either of the octahedral complexes, VO (*o*-i-Pr) (oxine)<sub>2</sub> of 2.317 (2) Å (Scheidt, 1973) or the average V–N distance found in [VO<sub>2</sub>EDTA]<sup>n-</sup>, (*n* = 1, 3), 2.360 Å (Scheidt, Collins & Hoard, 1971; Scheidt, Countryman & Hoard, 1971). The V–N(1) distance is similar to that found in other vanadyl complexes, as are V–O(2), V–O(4) and V–O(6) (Bruins & Weaver, 1970; Mathew *et al.*, 1970).

Bond lengths within the TTHA ligand are the same, within the errors, as those reported for Cr<sub>2</sub>TTHA.8H<sub>2</sub>O (Fallon & Gatehouse, 1974) and Cu<sub>2</sub>H<sub>2</sub>TTHA.7H<sub>2</sub>O

Table 4. Equations of least-squares planes and distances of individual atoms (Å) from the planes

$X$ ,  $Y$  and  $Z$  are coordinates in Å referred to an orthogonal system of axes having  $X$  along  $a$ ,  $Y$  in the  $ab$  plane and  $Z$  along  $c^*$ . Fractional coordinates  $x, y, z$  in the system are related to  $X, Y, Z$  by the matrix equation,

$$\begin{bmatrix} 10.003 & -5.387 & -2.119 \\ 0 & 13.898 & 0.711 \\ 0 & 0 & 6.242 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} X \\ Y \\ Z \end{bmatrix}$$

- (I) Plane through V, O(V), O(4), N(1), N(2)  
 $-0.5746X - 0.5449Y - 0.6107Z + 4.5592 = 0$   
 V 0.006 (1) O(4) -0.134 (5)  
 O(V) 0.115 (6) N(1) -0.118 (6)  
 N(2) 0.131 (6)
- (II) Plane through V, O(2), O(4), O(6), N(1)  
 $0.8156X - 0.4712Y - 0.3357Z + 6.9619 = 0$   
 V -0.315 (1) O(2) 0.022 (5)  
 N(1) 0.138 (6) O(4) 0.151 (6)  
 O(6) 0.004 (6)
- (III) Plane through V, O(V), O(2), O(6), N(2)  
 $0.1051X + 0.6727Y - 0.7324Z + 1.3838 = 0$   
 V -0.034 (1) O(2) 0.097 (5)  
 O(V) -0.073 (5) O(6) 0.087 (5)  
 N(2) -0.078 (5)
- (IV) Plane through O(2), O(4), O(6), N(1)  
 $0.8175X - 0.4671Y - 0.3369Z + 6.8755 = 0$   
 O(2) -0.061 (5) O(6) -0.070 (6)  
 O(4) 0.064 (6) N(1) 0.067 (6)  
 V -0.394 (1)
- (V) Plane through V, N(2), C(4), C(5), O(2)  
 $0.1883X + 0.6347Y - 0.7495Z + 1.9339 = 0$   
 V -0.069 (1) C(4) -0.091 (7)  
 N(2) 0.095 (5) C(5) 0.004 (7)  
 O(2) 0.061 (5)
- (VI) Plane through V, N(2), C(6), C(7), O(4)  
 V -0.180 (1) C(6) -0.256 (7)  
 N(2) 0.267 (6) C(7) 0.016 (8)  
 O(2) 0.152 (5)
- (VII) Plane through V, N(1), C(8), C(9), O(6)  
 V -0.148 (1) C(8) -0.161 (8)  
 N(1) 0.190 (6) C(9) -0.019 (8)  
 O(6) 0.138 (6)

(Leverett, 1974). A comparison of the angles in the glycinate rings, V-O(2)-C(5)-C(4)-N(2)-V and V-O(4)-C(7)-C(6)-N(2)-V, with the analogous rings in  $\text{Cr}_2\text{TTHA}\cdot 8\text{H}_2\text{O}$  shows that, because of the 0.39 Å displacement of the V atom from the O(2), O(4), O(6), N(1) plane, V-O(2)-C(5) and V-O(4)-C(7) have been substantially opened whilst O(2)-V-N(2) is closed and O(4)-V-N(2) is opened, the other glycinate ring angles being the same within the errors. Angles within the other glycinate ring are similar in both compounds.

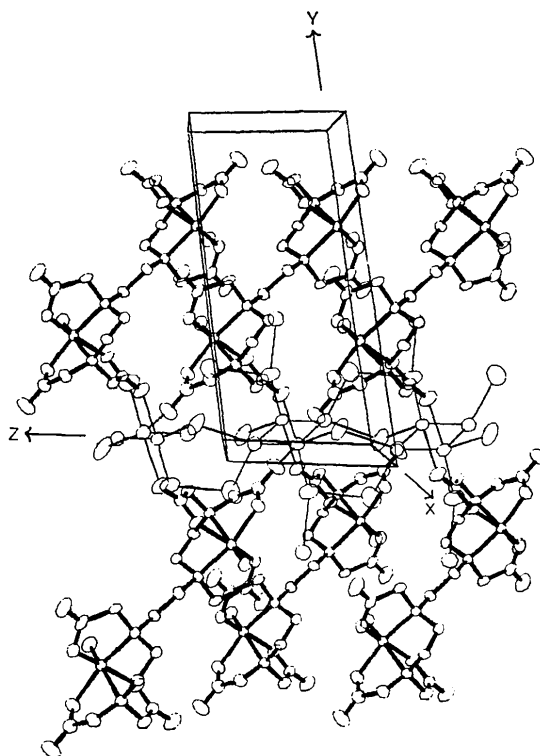


Fig. 3. The cell contents of the title compound.  $\text{Na}^+$  coordination and hydrogen bonding are delineated by thin lines. H atoms have been omitted for clarity.

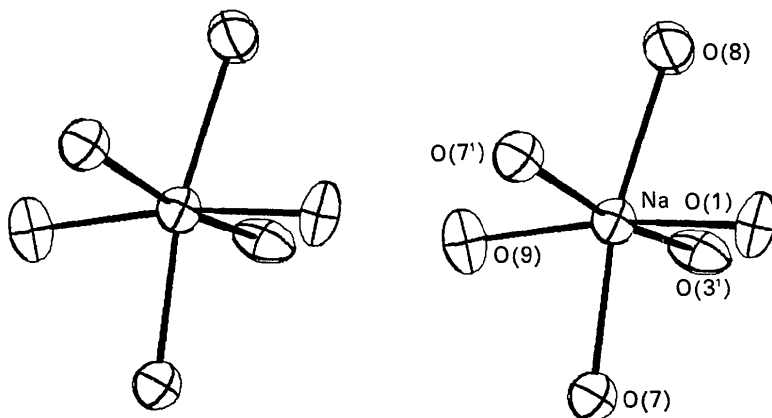


Fig. 4.  $\text{Na}^+$  ion coordination.

An analysis of the strain within the glycinate rings reveals that the equatorial ring is more strained than the axial rings; the sums of the interior angles, which are considered to be a qualitative guide to this strain (Park, Glick & Hoard, 1969), are respectively 525.4 and 532.4, 538.1°. The displacement of the V atom from the O(2), O(4), O(6), N(1) plane introduces more strain than is normal in the axial ring V–N(1)–C(8)–C(6)–O(6)–V, as is evidenced by the slightly reduced interior angle sum, 532.4°. Table 4 gives the displacement of atoms from the mean planes of these rings. All the acetate groups were found to be planar within experimental error.

The conformation of the ethylenediamine bridge is expressed by the N–C–C–N torsion angle of 56.2°, which is exactly that found in the Cr<sub>2</sub>TTHA complex (Fallon & Gatehouse, 1974). C(2) and C(3) are on opposite sides of the V, N(1), N(2) plane and respectively 0.248 (7) and 0.444 (7) Å from this plane. Bond distances and angles in the bridging ethylenediamine group [C(1)–C(1'), 1.543 (11), C(1)–N(1), 1.496 (9) Å and C(1')–C(1)–N(1), 113.4 (7)°] are the same, within experimental error, as those found in Cr<sub>2</sub>TTHA·8H<sub>2</sub>O.

A stereoscopic view of the unit-cell contents is given in Fig. 3. The Na<sup>+</sup> ion is in a slightly distorted octahedral environment, Fig. 4, the coordination lengths varying from 2.356 to 2.481 Å (Table 5). Possible hydrogen-bonding distances are also included in Table 5, these distances varying between 2.746 and 2.988 Å. By the criteria of Hamilton & Ibers (1968) the most likely hydrogen bond is where the O···O contact distance is *ca* 2.7 Å or less. A far stronger indication of hydrogen bonding is a marked shortening of the H···O van der Waals contact distance of *ca* 2.6 Å to *ca* 1.7 Å (Hamilton & Ibers, 1968), this being impossible to determine in the present case because of the uncertainty in the location of H atoms of the water molecules. These tentative hydrogen bonds and the Na coordination are depicted by thin lines in Fig. 3.

The observation of a magnetic exchange interaction by Smith *et al.* (1974) in the dinuclear TTHA chelate in solution was considered to be unusual, as previous explanations of this phenomenon were in terms of the delocalization of the unpaired electrons of the metal ions through a polyatomic bridging group involving some degree of multiple bonding (Hasty, Colburn & Hendrickson, 1973). It was also considered unlikely that any conformation the complex could adopt in solution would be such that close proximity of vanadyl

ions would allow direct overlap of the metal ion orbitals. The solution of the structure in the solid state apparently sheds no light on this subject as the intramolecular V–V contact distance of 7.482 Å cannot allow metal orbital overlap, and delocalization through the  $\sigma$  bridging system is unlikely. Exchange coupling through an intermolecular route is considered very implausible in aqueous solution.

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Table 5. *Hydrogen-bond distances and Na<sup>+</sup> coordination distances (Å)*

O(9)—O(11)	2.746	Na—O(1)	2.356
O(7)—O(10)	2.785	Na—O(3)	2.359
O(9)—O(10)	2.825	Na—O(9)	2.364
O(11)—O(5)	2.826	Na—O(7)	2.447
O(9)—O(1)	2.929	Na—O(7)	2.455
O(8)—O(4)	2.958	Na—O(8)	2.481
O(7)—O(8)	2.983		
O(11)—O(5)	2.988		