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(2,2′-Bipyridyl)bis(pentane-2,4-dionato)vanadium(III) perchlorate dichloromethane solvate

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.105
Data-to-parameter ratio = 18.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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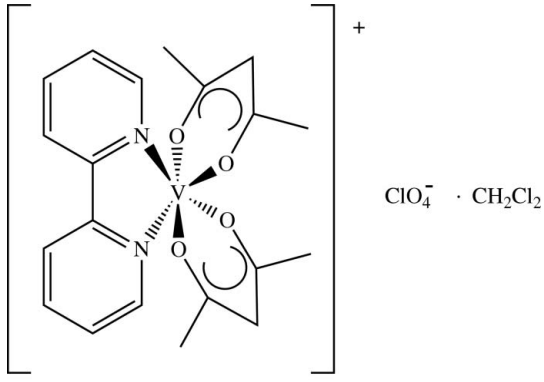
The title compound is a stoichiometrically solvated salt, $[V(C_5H_7O_2)_2(C_{10}H_8N_2)]ClO_4\cdot CH_2Cl_2$. The ionic components are linked by three C—H···O hydrogen bonds into chains from which the solvent dichloromethane molecules are pendant, and pairs of antiparallel (inversion-related) chains are linked by a single π–π stacking interaction.

Comment

The nitrogen heterocycles 1,10-phenanthroline (phen) and 2,2′-bipyridine (bipy) are among the most widely utilized chelating ligands in coordination chemistry (Lever, 2003). We have recently prepared mixed-ligand vanadium(III) complexes containing both pentane-2,4-dionate (also called acetylacetonate; acac) and 1,10-phenanthroline ligands (Kavitha *et al.*, 2006) in order to assess their antidiabetic activity. Although phen and bipy have similar structures, there is a difference in their chelating ability, which has been attributed to the difference in the geometry of the free molecules (Reyzer & Brodbelt, 1999; Oresmaa *et al.*, 2002). The title complex, (I), which contains a 2,2′-bipyridine ligand, has been prepared in order to compare its structure with that of the 1,10-phenanthroline analogue and with the longer term aim of testing its antidiabetic activity.



(I)

In the cation, which has approximate twofold rotational symmetry, the V atom is octahedrally coordinated (Table 1) by three bidentate ligands (two acac and one bipy): each cation is thus chiral. The cation in the arbitrarily chosen asymmetric unit (Fig. 1) has a Δ configuration, but space-group symmetry generates a racemic mixture of Λ and Δ enantiomers. The component species are linked by three independent two-centre C—H···O hydrogen bonds and one planar three-centre C—H···$(O)_2$ hydrogen bond (Table 2). One further C—H···O hydrogen bond links the ionic aggregates into a

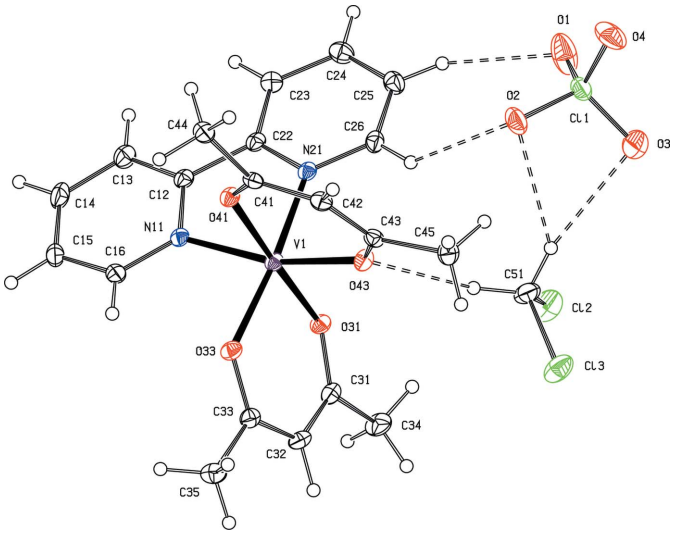


Figure 1
The asymmetric unit of (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). The C—H···O interactions are indicated by dashed lines.

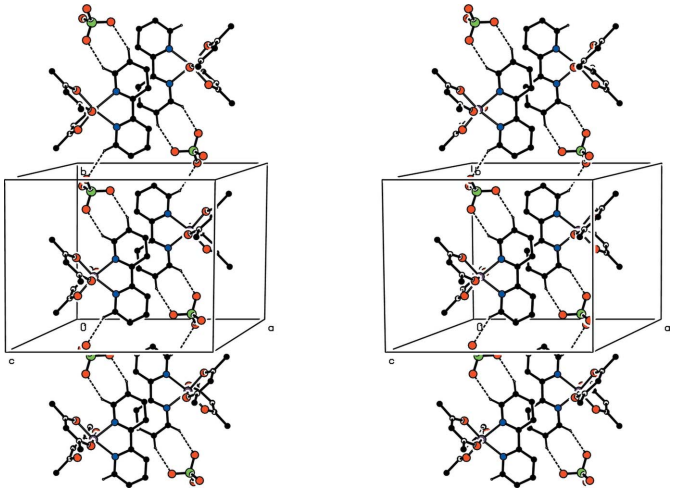


Figure 2
A stereoview of part of the crystal structure of (I), showing the formation of a π-stacked pair of hydrogen-bonded (dashed lines) chains. For clarity, the dichloromethane molecules have been omitted, as have the H atoms not involved in the hydrogen-bonding motifs shown.

$C(10)C(11)[R_2^2(7)]$ (Bernstein *et al.*, 1995) chain of rings running parallel to the [010] direction (Fig. 2); the dichloromethane molecules are pendant from this chain.

A single π–π stacking interaction links antiparallel pairs of these chains (Fig. 2). The rings (N21/C22–C26) in the cations at (x, y, z) and $(1-x, 1-y, 1-z)$ are strictly parallel, with an interplanar spacing of 3.426 (2) Å: the corresponding ring-centroid separation is 3.751 (2) Å, and the ring offset is 1.527 (2) Å. Similar C—H···O and π–π interactions were identified in the structure of the analogous phen complex $[V(acac)_2(phen)]ClO_4$ (Kavitha *et al.*, 2006). Otherwise, the bond lengths and angles of (I) present no unusual features, and they are very similar to those in the analogous phen complex.

Experimental

A solution of tris(pentane-2,4-dionato)vanadium(III) (0.30 g) and 2,2′-bipyridinium perchlorate (0.22 g) in methanol (30 ml) was heated under reflux for 3 h under an atmosphere of dinitrogen. The mixture was cooled to yield an orange solid which was crystallized by vapour diffusion of light petroleum into a solution in dichloromethane (m.p. 480 K).

Crystal data

$[V(C_5H_7O_2)_2(C_{10}H_8N_2)]$-$ClO_4\cdot CH_2Cl_2$
M_r = 589.71
Monoclinic, $P2_1/c$
a = 15.0676 (5) Å
b = 12.5534 (3) Å
c = 14.5533 (5) Å
β = 111.4860 (13)°
V = 2561.45 (14) Å^3
Z = 4
D_x = 1.529 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5869 reflections
θ = 3.2–27.5°
μ = 0.75 mm^{-1}
T = 120 (2) K
Plate, orange
0.50 × 0.20 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.706, T_{max} = 0.956
37694 measured reflections
5869 independent reflections
4242 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 27.5°
$h = -19 \rightarrow 19$
$k = -16 \rightarrow 16$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.105
S = 1.07
5869 reflections
320 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 2.8417P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected bond lengths (Å).

V1—O33	1.9487 (17)	V1—O31	1.9779 (17)
V1—O43	1.9526 (17)	V1—N11	2.116 (2)
V1—O41	1.9694 (16)	V1—N21	2.125 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O4^{i}	0.95	2.51	3.349 (4)	147
C25—H25···O1	0.95	2.41	3.285 (4)	153
C26—H26···O2	0.95	2.47	3.249 (3)	139
C51—H51*A*···O43	0.99	2.53	3.429 (4)	150
C51—H51*B*···O2	0.99	2.59	3.404 (4)	140
C51—H51*B*···O3	0.99	2.44	3.397 (4)	161

Symmetry code: (i) $x, y+1, z$.

All H atoms were located in a difference map and then treated as riding atoms, with C—H = 0.95 (ring H), 0.98 (methyl H) or 0.99 Å (CH_2), and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduc-

tion: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. The authors thank the staff for all their help and advice.

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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.0676$ (5) Å
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$\beta = 111.4860$ (13)°
$V = 2561.45$ (14) Å^3
$Z = 4$
$F(000) = 1208$
$D_x = 1.529$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5869 reflections
$\theta = 3.2$–27.5°
$\mu = 0.75$ mm^{-1}
$T = 120$ K
Plate, orange
0.50 × 0.20 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: Bruker–Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.706$, $T_{max} = 0.956$
37694 measured reflections
5869 independent reflections
4242 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -19\rightarrow19$
$k = -16\rightarrow16$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.105$
$S = 1.07$
5869 reflections
320 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 2.8417P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
V1	0.71091 (3)	0.62674 (3)	0.40436 (3)	0.01887 (11)
N11	0.59056 (14)	0.72637 (16)	0.37634 (14)	0.0191 (4)
C12	0.50629 (17)	0.67768 (19)	0.36333 (18)	0.0209 (5)
C13	0.42284 (19)	0.7349 (2)	0.3421 (2)	0.0302 (6)
C14	0.4254 (2)	0.8446 (2)	0.3349 (2)	0.0335 (7)
C15	0.51090 (19)	0.8947 (2)	0.34727 (19)	0.0276 (6)
C16	0.59128 (19)	0.8328 (2)	0.36672 (18)	0.0228 (5)
N21	0.59971 (14)	0.51845 (16)	0.39565 (14)	0.0201 (4)
C22	0.51166 (17)	0.56069 (19)	0.37491 (17)	0.0208 (5)
C23	0.43394 (19)	0.4968 (2)	0.36685 (19)	0.0258 (6)
C24	0.4470 (2)	0.3880 (2)	0.3813 (2)	0.0300 (6)
C25	0.5367 (2)	0.3449 (2)	0.4029 (2)	0.0289 (6)
C26	0.61101 (19)	0.4125 (2)	0.40911 (18)	0.0245 (5)
C31	0.81839 (18)	0.6627 (2)	0.61603 (18)	0.0233 (5)
O31	0.74506 (12)	0.62160 (13)	0.54909 (12)	0.0224 (4)
C32	0.87980 (17)	0.7349 (2)	0.59678 (19)	0.0253 (6)
C33	0.86659 (17)	0.7763 (2)	0.50439 (19)	0.0229 (5)
O33	0.79843 (12)	0.74640 (13)	0.42470 (12)	0.0234 (4)
C34	0.8345 (2)	0.6315 (2)	0.72030 (19)	0.0351 (7)
C35	0.9308 (2)	0.8620 (2)	0.4930 (2)	0.0317 (6)
C41	0.71562 (17)	0.58255 (19)	0.20685 (18)	0.0203 (5)
O41	0.67408 (12)	0.62704 (13)	0.25980 (12)	0.0213 (4)
C42	0.79325 (18)	0.51384 (19)	0.24419 (19)	0.0230 (5)
C43	0.83089 (17)	0.47996 (19)	0.34177 (19)	0.0213 (5)
O43	0.80044 (12)	0.51241 (14)	0.40936 (12)	0.0239 (4)
C44	0.6717 (2)	0.6036 (2)	0.09848 (19)	0.0273 (6)
C45	0.90869 (19)	0.3987 (2)	0.3743 (2)	0.0297 (6)
Cl1	0.73123 (5)	0.11454 (5)	0.42413 (5)	0.03025 (16)
O1	0.64206 (18)	0.11127 (18)	0.4379 (2)	0.0655 (8)
O2	0.74504 (15)	0.21793 (15)	0.38921 (16)	0.0391 (5)
O3	0.80694 (18)	0.09205 (18)	0.51596 (17)	0.0543 (6)
O4	0.73151 (19)	0.03468 (17)	0.35384 (17)	0.0530 (6)
C51	0.8670 (2)	0.3419 (3)	0.6071 (2)	0.0364 (7)
Cl2	0.82681 (6)	0.33110 (8)	0.70602 (6)	0.0493 (2)
Cl3	0.99178 (5)	0.35970 (7)	0.65157 (6)	0.0454 (2)
H13	0.3645	0.6993	0.3326	0.036*
H14	0.3689	0.8853	0.3216	0.040*
H15	0.5141	0.9700	0.3424	0.033*
H16	0.6497	0.8668	0.3736	0.027*
H23	0.3725	0.5273	0.3516	0.031*
H24	0.3946	0.3432	0.3763	0.036*
H25	0.5470	0.2705	0.4133	0.035*
H26	0.6727	0.3829	0.4235	0.029*
H32	0.9346	0.7572	0.6508	0.030*
H34A	0.8048	0.6842	0.7496	0.053*

H34B	0.9032	0.6284	0.7587	0.053*
H34C	0.8061	0.5614	0.7208	0.053*
H35A	0.9654	0.8356	0.4521	0.048*
H35B	0.9766	0.8823	0.5581	0.048*
H35C	0.8926	0.9242	0.4611	0.048*
H42	0.8222	0.4887	0.2003	0.028*
H44A	0.6035	0.5868	0.0749	0.041*
H44B	0.7027	0.5590	0.0637	0.041*
H44C	0.6801	0.6788	0.0857	0.041*
H45A	0.9596	0.4236	0.4344	0.044*
H45B	0.9344	0.3882	0.3221	0.044*
H45C	0.8831	0.3312	0.3877	0.044*
H51A	0.8354	0.4032	0.5650	0.044*
H51B	0.8497	0.2767	0.5662	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
V1	0.0197 (2)	0.0222 (2)	0.0139 (2)	0.00181 (17)	0.00524 (16)	−0.00108 (17)
N11	0.0223 (10)	0.0219 (10)	0.0122 (10)	0.0007 (8)	0.0053 (8)	0.0005 (8)
C12	0.0224 (12)	0.0245 (13)	0.0151 (12)	0.0016 (10)	0.0059 (10)	−0.0013 (10)
C13	0.0232 (13)	0.0322 (15)	0.0342 (16)	0.0042 (11)	0.0093 (12)	0.0014 (12)
C14	0.0297 (15)	0.0322 (15)	0.0347 (17)	0.0134 (12)	0.0073 (13)	0.0060 (12)
C15	0.0372 (15)	0.0211 (13)	0.0215 (14)	0.0071 (11)	0.0072 (12)	0.0013 (10)
C16	0.0307 (14)	0.0218 (12)	0.0152 (12)	−0.0016 (10)	0.0074 (11)	−0.0009 (10)
N21	0.0225 (10)	0.0224 (10)	0.0140 (10)	0.0028 (8)	0.0048 (9)	−0.0009 (8)
C22	0.0226 (12)	0.0246 (13)	0.0140 (12)	0.0016 (10)	0.0053 (10)	−0.0013 (10)
C23	0.0261 (13)	0.0274 (13)	0.0248 (14)	−0.0007 (11)	0.0104 (11)	−0.0010 (11)
C24	0.0328 (15)	0.0299 (15)	0.0299 (15)	−0.0067 (12)	0.0147 (12)	−0.0027 (12)
C25	0.0386 (15)	0.0232 (13)	0.0258 (15)	−0.0009 (11)	0.0128 (13)	0.0015 (11)
C26	0.0294 (14)	0.0232 (12)	0.0198 (13)	0.0057 (10)	0.0076 (11)	0.0018 (10)
C31	0.0237 (13)	0.0282 (13)	0.0172 (13)	0.0078 (10)	0.0065 (11)	−0.0017 (10)
O31	0.0238 (9)	0.0270 (9)	0.0153 (9)	0.0007 (7)	0.0060 (7)	−0.0010 (7)
C32	0.0189 (12)	0.0337 (14)	0.0192 (13)	0.0007 (10)	0.0021 (10)	−0.0039 (11)
C33	0.0193 (12)	0.0255 (13)	0.0235 (14)	0.0037 (10)	0.0073 (11)	−0.0038 (10)
O33	0.0229 (9)	0.0288 (9)	0.0169 (9)	−0.0018 (7)	0.0053 (7)	0.0004 (7)
C34	0.0400 (16)	0.0447 (17)	0.0164 (14)	−0.0031 (13)	0.0053 (12)	0.0008 (12)
C35	0.0288 (14)	0.0369 (16)	0.0277 (15)	−0.0083 (12)	0.0084 (12)	−0.0026 (12)
C41	0.0243 (12)	0.0189 (12)	0.0179 (12)	−0.0062 (10)	0.0078 (10)	−0.0032 (10)
O41	0.0238 (9)	0.0251 (9)	0.0145 (8)	0.0027 (7)	0.0062 (7)	−0.0010 (7)
C42	0.0254 (13)	0.0240 (13)	0.0215 (13)	−0.0030 (10)	0.0109 (11)	−0.0038 (10)
C43	0.0190 (12)	0.0189 (12)	0.0268 (14)	−0.0029 (9)	0.0095 (11)	−0.0024 (10)
O43	0.0238 (9)	0.0281 (9)	0.0194 (9)	0.0064 (7)	0.0074 (8)	0.0012 (7)
C44	0.0391 (15)	0.0244 (13)	0.0179 (13)	−0.0025 (11)	0.0097 (12)	−0.0006 (10)
C45	0.0280 (14)	0.0284 (14)	0.0342 (16)	0.0060 (11)	0.0134 (12)	0.0002 (12)
Cl1	0.0368 (4)	0.0213 (3)	0.0326 (4)	−0.0015 (3)	0.0127 (3)	0.0009 (3)
O1	0.0581 (16)	0.0403 (13)	0.117 (2)	0.0093 (11)	0.0545 (17)	0.0239 (14)
O2	0.0507 (13)	0.0224 (10)	0.0452 (13)	−0.0033 (9)	0.0187 (11)	0.0070 (9)

O3	0.0660 (16)	0.0446 (13)	0.0385 (14)	0.0026 (12)	0.0028 (12)	0.0061 (10)
O4	0.0817 (17)	0.0329 (12)	0.0459 (14)	−0.0104 (12)	0.0252 (13)	−0.0161 (10)
C51	0.0273 (14)	0.0440 (17)	0.0299 (16)	−0.0083 (13)	0.0007 (13)	0.0040 (13)
Cl2	0.0371 (4)	0.0672 (5)	0.0473 (5)	0.0015 (4)	0.0198 (4)	0.0126 (4)
Cl3	0.0273 (4)	0.0657 (5)	0.0389 (4)	−0.0050 (3)	0.0070 (3)	0.0168 (4)

Geometric parameters (Å, º)

V1—O33	1.9487 (17)	C32—H32	0.95
V1—O43	1.9526 (17)	C33—O33	1.292 (3)
V1—O41	1.9694 (16)	C33—C35	1.496 (4)
V1—O31	1.9779 (17)	C34—H34A	0.98
V1—N11	2.116 (2)	C34—H34B	0.98
V1—N21	2.125 (2)	C34—H34C	0.98
N11—C16	1.343 (3)	C35—H35A	0.98
N11—C12	1.359 (3)	C35—H35B	0.98
C12—C13	1.381 (3)	C35—H35C	0.98
C12—C22	1.477 (3)	C41—O41	1.285 (3)
C13—C14	1.383 (4)	C41—C42	1.394 (3)
C13—H13	0.95	C41—C44	1.494 (3)
C14—C15	1.385 (4)	C42—C43	1.389 (4)
C14—H14	0.95	C42—H42	0.95
C15—C16	1.379 (4)	C43—O43	1.294 (3)
C15—H15	0.95	C43—C45	1.494 (3)
C16—H16	0.95	C44—H44A	0.98
N21—C26	1.347 (3)	C44—H44B	0.98
N21—C22	1.356 (3)	C44—H44C	0.98
C22—C23	1.389 (3)	C45—H45A	0.98
C23—C24	1.385 (4)	C45—H45B	0.98
C23—H23	0.95	C45—H45C	0.98
C24—C25	1.380 (4)	Cl1—O1	1.430 (2)
C24—H24	0.95	Cl1—O3	1.432 (2)
C25—C26	1.381 (4)	Cl1—O4	1.433 (2)
C25—H25	0.95	Cl1—O2	1.4366 (19)
C26—H26	0.95	C51—Cl2	1.759 (3)
C31—O31	1.284 (3)	C51—Cl3	1.765 (3)
C31—C32	1.395 (4)	C51—H51A	0.99
C31—C34	1.498 (4)	C51—H51B	0.99
C32—C33	1.386 (4)		

O33—V1—O43	98.11 (7)	C33—C32—C31	124.6 (2)
O33—V1—O41	94.07 (7)	C33—C32—H32	117.7
O43—V1—O41	87.81 (7)	C31—C32—H32	117.7
O33—V1—O31	88.04 (7)	O33—C33—C32	123.1 (2)
O43—V1—O31	91.70 (7)	O33—C33—C35	116.3 (2)
O41—V1—O31	177.88 (7)	C32—C33—C35	120.6 (2)
O33—V1—N11	93.33 (7)	C33—O33—V1	129.18 (16)
O43—V1—N11	166.71 (8)	C31—C34—H34A	109.5

O41—V1—N11	84.65 (7)	C31—C34—H34B	109.5
O31—V1—N11	95.44 (7)	H34A—C34—H34B	109.5
O33—V1—N21	167.72 (7)	C31—C34—H34C	109.5
O43—V1—N21	92.92 (7)	H34A—C34—H34C	109.5
O41—V1—N21	91.72 (7)	H34B—C34—H34C	109.5
O31—V1—N21	86.25 (7)	C33—C35—H35A	109.5
N11—V1—N21	76.43 (8)	C33—C35—H35B	109.5
C16—N11—C12	118.4 (2)	H35A—C35—H35B	109.5
C16—N11—V1	124.66 (17)	C33—C35—H35C	109.5
C12—N11—V1	116.88 (15)	H35A—C35—H35C	109.5
N11—C12—C13	121.7 (2)	H35B—C35—H35C	109.5
N11—C12—C22	115.0 (2)	O41—C41—C42	124.0 (2)
C13—C12—C22	123.3 (2)	O41—C41—C44	115.6 (2)
C12—C13—C14	119.1 (3)	C42—C41—C44	120.3 (2)
C12—C13—H13	120.5	C41—O41—V1	129.15 (16)
C14—C13—H13	120.5	C43—C42—C41	123.9 (2)
C13—C14—C15	119.6 (2)	C43—C42—H42	118.0
C13—C14—H14	120.2	C41—C42—H42	118.0
C15—C14—H14	120.2	O43—C43—C42	123.7 (2)
C16—C15—C14	118.4 (2)	O43—C43—C45	115.4 (2)
C16—C15—H15	120.8	C42—C43—C45	120.8 (2)
C14—C15—H15	120.8	C43—O43—V1	129.45 (16)
N11—C16—C15	122.8 (2)	C41—C44—H44A	109.5
N11—C16—H16	118.6	C41—C44—H44B	109.5
C15—C16—H16	118.6	H44A—C44—H44B	109.5
C26—N21—C22	118.7 (2)	C41—C44—H44C	109.5
C26—N21—V1	124.64 (17)	H44A—C44—H44C	109.5
C22—N21—V1	116.67 (16)	H44B—C44—H44C	109.5
N21—C22—C23	121.3 (2)	C43—C45—H45A	109.5
N21—C22—C12	115.0 (2)	C43—C45—H45B	109.5
C23—C22—C12	123.8 (2)	H45A—C45—H45B	109.5
C24—C23—C22	119.2 (2)	C43—C45—H45C	109.5
C24—C23—H23	120.4	H45A—C45—H45C	109.5
C22—C23—H23	120.4	H45B—C45—H45C	109.5
C25—C24—C23	119.6 (2)	O1—Cl1—O3	109.39 (17)
C25—C24—H24	120.2	O1—Cl1—O4	109.18 (16)
C23—C24—H24	120.2	O3—Cl1—O4	108.58 (15)
C24—C25—C26	118.5 (2)	O1—Cl1—O2	109.92 (13)
C24—C25—H25	120.8	O3—Cl1—O2	109.82 (13)
C26—C25—H25	120.8	O4—Cl1—O2	109.92 (14)
N21—C26—C25	122.7 (2)	Cl2—C51—Cl3	110.46 (16)
N21—C26—H26	118.6	Cl2—C51—H51A	109.6
C25—C26—H26	118.6	Cl3—C51—H51A	109.6
O31—C31—C32	124.0 (2)	Cl2—C51—H51B	109.6
O31—C31—C34	116.0 (2)	Cl3—C51—H51B	109.6
C32—C31—C34	120.0 (2)	H51A—C51—H51B	108.1
C31—O31—V1	127.66 (16)		

O33—V1—N11—C16	7.3 (2)	C12—C22—C23—C24	−178.5 (2)
O43—V1—N11—C16	−142.2 (3)	C22—C23—C24—C25	−0.3 (4)
O41—V1—N11—C16	−86.47 (19)	C23—C24—C25—C26	−0.3 (4)
O31—V1—N11—C16	95.65 (19)	C22—N21—C26—C25	−0.2 (4)
N21—V1—N11—C16	−179.6 (2)	V1—N21—C26—C25	179.91 (19)
O33—V1—N11—C12	−175.51 (17)	C24—C25—C26—N21	0.5 (4)
O43—V1—N11—C12	35.0 (4)	C32—C31—O31—V1	11.5 (3)
O41—V1—N11—C12	90.70 (17)	C34—C31—O31—V1	−170.41 (17)
O31—V1—N11—C12	−87.17 (17)	O33—V1—O31—C31	−18.4 (2)
N21—V1—N11—C12	−2.37 (16)	O43—V1—O31—C31	79.7 (2)
C16—N11—C12—C13	−0.9 (3)	N11—V1—O31—C31	−111.5 (2)
V1—N11—C12—C13	−178.30 (19)	N21—V1—O31—C31	172.5 (2)
C16—N11—C12—C22	179.8 (2)	O31—C31—C32—C33	4.1 (4)
V1—N11—C12—C22	2.5 (3)	C34—C31—C32—C33	−174.0 (2)
N11—C12—C13—C14	−0.6 (4)	C31—C32—C33—O33	−4.8 (4)
C22—C12—C13—C14	178.5 (2)	C31—C32—C33—C35	173.5 (2)
C12—C13—C14—C15	1.2 (4)	C32—C33—O33—V1	−10.6 (3)
C13—C14—C15—C16	−0.1 (4)	C35—C33—O33—V1	171.11 (17)
C12—N11—C16—C15	2.1 (4)	O43—V1—O33—C33	−73.3 (2)
V1—N11—C16—C15	179.19 (18)	O41—V1—O33—C33	−161.68 (19)
C14—C15—C16—N11	−1.5 (4)	O31—V1—O33—C33	18.1 (2)
O33—V1—N21—C26	−144.0 (3)	N11—V1—O33—C33	113.5 (2)
O43—V1—N21—C26	9.9 (2)	N21—V1—O33—C33	80.4 (4)
O41—V1—N21—C26	97.8 (2)	C42—C41—O41—V1	6.9 (3)
O31—V1—N21—C26	−81.62 (19)	C44—C41—O41—V1	−176.63 (16)
N11—V1—N21—C26	−178.1 (2)	O33—V1—O41—C41	84.82 (19)
O33—V1—N21—C22	36.0 (4)	O43—V1—O41—C41	−13.15 (19)
O43—V1—N21—C22	−170.05 (17)	N11—V1—O41—C41	177.8 (2)
O41—V1—N21—C22	−82.15 (17)	N21—V1—O41—C41	−106.01 (19)
O31—V1—N21—C22	98.44 (17)	O41—C41—C42—C43	4.4 (4)
N11—V1—N21—C22	1.92 (16)	C44—C41—C42—C43	−171.9 (2)
C26—N21—C22—C23	−0.4 (3)	C41—C42—C43—O43	−3.2 (4)
V1—N21—C22—C23	179.52 (18)	C41—C42—C43—C45	174.5 (2)
C26—N21—C22—C12	178.8 (2)	C42—C43—O43—V1	−9.4 (3)
V1—N21—C22—C12	−1.3 (3)	C45—C43—O43—V1	172.80 (16)
N11—C12—C22—N21	−0.8 (3)	O33—V1—O43—C43	−79.4 (2)
C13—C12—C22—N21	180.0 (2)	O41—V1—O43—C43	14.4 (2)
N11—C12—C22—C23	178.4 (2)	O31—V1—O43—C43	−167.7 (2)
C13—C12—C22—C23	−0.8 (4)	N11—V1—O43—C43	69.7 (4)
N21—C22—C23—C24	0.6 (4)	N21—V1—O43—C43	106.0 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O4^{i}	0.95	2.51	3.349 (4)	147
C25—H25···O1	0.95	2.41	3.285 (4)	153
C26—H26···O2	0.95	2.47	3.249 (3)	139
C51—H51*A*···O43	0.99	2.53	3.429 (4)	150

C51—H51*B*···O2	0.99	2.59	3.404 (4)	140
C51—H51*B*···O3	0.99	2.44	3.397 (4)	161

Symmetry code: (i) *x*, *y*+1, *z*.