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Tris[(3-aminopropyl)dimethylammonium] decavanadate(V) hexahydrate

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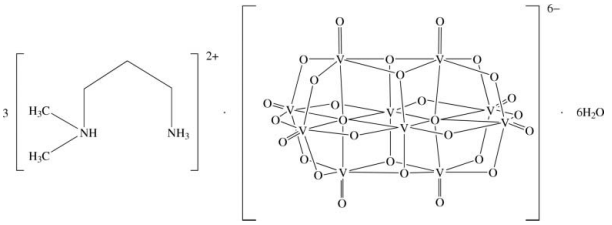
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.045; wR factor = 0.134; data-to-parameter ratio = 13.6.

The title compound, $3(C_5H_{16}N_2)^{2+}\cdot[V_{10}O_{28}]^{6-}\cdot 6H_2O$, consists of decavanadate polyanions, doubly protonated *N*,*N*-dimethylpropane-1,3-diammonium cations (H_2dmpn^{2+}) and uncoordinated water molecules. Two crystallographically independent decavanadate anions are located across inversion centers. The terminal V=O bond distances are much shorter than the bridging V—O bond distances. The structural components are linked by extensive hydrogen bonding, forming a three-dimension supramolecular architecture.

Related literature

For general background, see Boyd *et al.* (1985); Csermely *et al.* (1985); DeMaster & Mitchell (1973); Pai *et al.* (1977); Soman *et al.* (1983). For related structures, see Correia *et al.* (2004); Fratzky *et al.* (2000); Gong *et al.* (2006). For synthesis, see Sathyanarayana & Patel (1965).



Experimental

Crystal data

$3(C_5H_{16}N_2)^{2+}\cdot[V_{10}O_{28}]^{6-}\cdot 6H_2O$
M_r = 1378.09
Triclinic, $P\overline{1}$
a = 11.525 (2) Å
b = 11.743 (2) Å
c = 18.709 (4) Å
α = 90.45 (3)°
β = 94.21 (3)°
γ = 117.29 (3)°
V = 2241.7 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.09 mm^{-1}
T = 298 (2) K
0.30 × 0.26 × 0.18 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.556, T_{max} = 0.684
12138 measured reflections
8110 independent reflections
4858 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.134
S = 1.03
8110 reflections
595 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.02 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

Table 1
Selected bond lengths (Å).

V1—O1	1.612 (3)	V6—O15	1.617 (3)
V2—O2	1.622 (3)	V7—O16	1.605 (3)
V3—O3	1.614 (3)	V8—O17	1.612 (4)
V4—O4	1.603 (3)	V9—O18	1.602 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O13^{i}	0.91	1.79	2.691 (5)	173
N2—H2D···O32W	0.89	2.08	2.968 (7)	172
N2—H2E···O9^{ii}	0.89	2.05	2.873 (5)	153
N2—H2F···O6^{iii}	0.89	1.89	2.772 (6)	173
N3—H3···O27^{iv}	0.91	1.87	2.736 (6)	159
N4—H4C···O20^{v}	0.89	1.89	2.772 (5)	171
N4—H4D···O33W^{vi}	0.89	2.21	3.035 (7)	154
N4—H4E···O23	0.89	1.99	2.820 (5)	156
N5—H5···O26	0.91	1.82	2.709 (5)	166
N6—H6D···O17	0.89	2.34	3.056 (6)	137
N6—H6D···O32W^{vii}	0.89	2.50	3.046 (7)	120
N6—H6E···O31W^{viii}	0.89	1.89	2.745 (6)	160
N6—H6F···O2^{vii}	0.89	2.12	2.958 (6)	156
O29W—H29A···O1	0.91	2.00	2.848 (5)	154
O29W—H29B···O8^{ii}	0.94	1.90	2.790 (5)	156
O30W—H30A···O3^{vii}	0.84	2.06	2.895 (5)	174
O30W—H30B···O7^{ix}	0.87	1.86	2.716 (5)	173
O31W—H31A···O21	0.95	1.83	2.770 (5)	173
O31W—H31B···O30W	0.82	1.94	2.724 (6)	160
O32W—H32A···O29W	0.88	2.00	2.808 (6)	152
O32W—H32B···O34W^{ix}	0.88	2.03	2.873 (8)	160
O33W—H33A···O15^{x}	0.87	1.98	2.787 (6)	153
O33W—H33B···O22^{vi}	0.97	1.84	2.723 (5)	150
O34W—H34A···O18	0.97	2.11	3.055 (7)	163
O34W—H34B···O33W^{vi}	0.80	2.24	2.903 (8)	141

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $x, y+1, z$; (iii) $x+1, y+1, z$; (iv) $-x, -y, -z$; (v) $x+1, y, z$; (vi) $-x, -y+1, -z$; (vii) $-x, -y+1, -z+1$; (viii) $x-1, y, z$; (ix) $-x+1, -y+1, -z+1$; (x) $-x, -y+2, -z$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2250).

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supplementary materials

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Tris[(3-aminopropyl)dimethylammonium] decavanadate(V) hexahydrate

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Comment

Decavanadate has shown high affinity for selected kinases, phosphorylase and reverse transcriptase and has been used to facilitate crystallization of proteins (Boyd *et al.*, 1985; Csermely *et al.*, 1985; DeMaster & Mitchell, 1973; Pai *et al.*, 1977; Soman *et al.*, 1983). Herein, we report the structure of a three-dimensional supramolecular assembly based on decavanadate, *N*,*N*-dimethylpropane-1,3-diammonium (H_2dmpn^{2+}) and lattice water molecule building blocks, formulated as $3(C_5H_{16}N_2)^{2+}\cdot(V_{10}O_{28})^{6-}\cdot 6H_2O$, (I).

The molecular structure of (I) comprises decavanadate polyanions, H_2dmpn^{2+} cations and lattice water molecules in a stoichiometric ratio of 1:3:6 (Fig. 1). There are two halves of independent $[V_{10}O_{28}]^{6-}$ ions, located on different inversion centers and exhibit the usual structure consisting in a stacking of ten octahedra (Correia *et al.*, 2004; Fratzky *et al.*, 2000; Gong *et al.*, 2006). The terminal O—V bond distances are much shorter than bridging O—V bond distances (Table 1). All the H_2dmpn^{2+} cations adopt anti-anti conformations, with N···N separations of 4.992 (7) Å (N1···N2), 4.994 (7) Å (N3···N4) and 4.973 (7) Å (N5···N6), respectively.

The most noticeable feature of the title compound is its extensive hydrogen bond network between the structural components (Table 2). Viewed along *c* axis, the H_2dmpn^{2+} cations containing atoms N1 and N2, the decavanadate ions incorporating atoms V1 to V5, O29W and O30W are involved in two-dimensional hydrogen-bonding networks (Fig. 2), which interleave with other parallel networks formed by the H_2dmpn^{2+} cations containing atoms N3 and N4, the other kind decavanadate ions, O33W and O34W (Fig. 3). Then these two kinds of decavanadate anions are both further connected by the H_2dmpn^{2+} cations containing atoms N5 and N6, O31W and O32W (Fig. 4), resulting in a three-dimensional supramolecular architecture.

Experimental

A solution of oxovanadium(IV) oxalate dihydrate (0.095 g, 0.5 mmol), prepared according to the literature procedure (Sathyanarayana & Patel, 1965), in 95% methanol (12 ml) was added successively to a solution of *N*,*N*-dimethylpropane-1,3-diamine (0.051 g, 0.5 mmol) in methanol (5 ml). The mixture was stirred continuously at 333 K for 6 h and a lot of brown precipitate formed. The precipitate was filtered, washed sequentially with methanol and diethyl ether, and then dissolved in water. Orange single crystals of (I) (55% yield based on vanadium) suitable for X-ray analysis were obtained from the aqueous solution by slow evaporation at room temperature. Elemental analysis calculated: C 13.07, H 4.39, N 6.10%; found: C 13.36, H 4.51, N 5.87%.

Refinement

H atoms of water molecules were located in a difference Fourier map and were refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(O). Other H atoms were placed in calculated positions, with C—H = 0.97 Å (methylene) or 0.96 Å (methyl) and N—H = 0.89 Å (protonated primary ammonium) or 0.91 Å (protonated tertiary ammonium), and included in the final cycles of refinement in riding mode, with U_{iso}(H) = 1.5U_{eq}(C,*N*) for methyl and protonated primary ammonium and 1.2U_{eq}(C,*N*) for others.

Figures

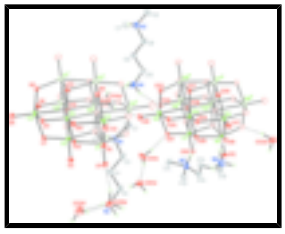

Fig. 1. A view of (I) with the atomic numbering scheme. Full displacement ellipsoids (for the independent moiety) and open ellipsoids (for the symmetry-related part) are drawn at the 30% probability level. C-bound H atoms have been omitted for clarity. Dashed lines indicate hydrogen bonds. [Symmetry codes: (i) −*x*, −*y*, −*z* + 1; (ii) −*x*, −*y* + 1, −*z*.]

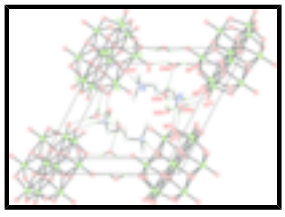

Fig. 2. The two-dimensional hydrogen-bonded network formed by the H_2dmpn^{2+} cations containing atoms N1 and N2, the decavanadate ions incorporating atoms V1 to V5 and water molecules, viewed along *c* axis. [Symmetry codes: (i) −*x*, −*y*, −*z* + 1; (iii) *x*, *y* + 1, *z*; (iv) *x* + 1, *y* + 1, *z*; (vii) −*x*, −*y* + 1, −*z* + 1; (ix) −*x* + 1, −*y* + 1, −*z* + 1.]

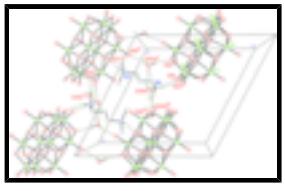

Fig. 3. The two-dimensional hydrogen-bonded network formed by the H_2dmpn^{2+} cations containing atoms N3 and N4, the decavanadate ions incorporating atoms V6 to V10 and water molecules, viewed along *c* axis. [Symmetry codes: (ii) −*x*, −*y* + 1, −*z*; (v) −*x*, −*y*, −*z*; (vi) *x* + 1, *y*, *z*; (ix) −*x* + 1, −*y* + 1, −*z* + 1; (xi) *x*, *y* − 1, *z*.]

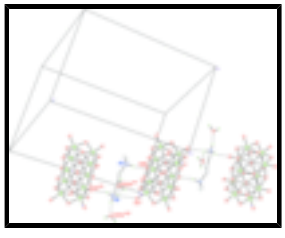

Fig. 4. The intermolecular hydrogen bonds between the H_2dmpn^{2+} cations containing atoms N5 and N6, both two kinds of decavanadate anions and water molecules. [Symmetry codes: (vii) −*x*, −*y* + 1, −*z* + 1; (viii) *x* − 1, *y*, *z*.]

Tris[(3-aminopropyl)dimethylammonium] decavanadate(V) hexahydrate

Crystal data

$3(C_5H_{16}N_2)^{2+}.[V_{10}O_{28}]^{6-}.6H_2O$	$Z = 2$
$M_r = 1378.09$	$F_{000} = 1388$
Triclinic, $P\overline{1}$	$D_x = 2.042$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å

a = 11.525 (2) Å	Cell parameters from 1736 reflections
b = 11.743 (2) Å	θ = 3.5–25.1º
c = 18.709 (4) Å	μ = 2.09 mm^{-1}
α = 90.45 (3)º	T = 298 (2) K
β = 94.21 (3)º	Block, orange
γ = 117.29 (3)º	0.30 × 0.26 × 0.18 mm
V = 2241.7 (10) $Å^3$	

Data collection

Bruker APEX area-detector diffractometer	8110 independent reflections
Radiation source: fine-focus sealed tube	4858 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
T = 298(2) K	θ_{max} = 25.2º
φ and ω scan	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -13 \rightarrow 13$
T_{min} = 0.556, T_{max} = 0.684	$k = -14 \rightarrow 11$
12138 measured reflections	$l = -19 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.134	$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 1.1434P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
8110 reflections	$\Delta\rho_{max}$ = 1.02 e $Å^{-3}$
595 parameters	$\Delta\rho_{min}$ = −0.71 e $Å^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1582 (6)	0.3274 (6)	0.3030 (3)	0.0486 (17)
H1A	0.1923	0.3863	0.2656	0.073*
H1B	0.0723	0.3159	0.3111	0.073*
H1C	0.1532	0.2464	0.2891	0.073*
C2	0.3772 (6)	0.3895 (6)	0.3602 (3)	0.0495 (17)
H2A	0.3684	0.3055	0.3500	0.074*
H2B	0.4341	0.4263	0.4032	0.074*
H2C	0.4137	0.4430	0.3210	0.074*
C3	0.2530 (6)	0.5035 (5)	0.3935 (3)	0.0396 (15)
H3A	0.1647	0.4905	0.3986	0.047*
H3B	0.2879	0.5636	0.3560	0.047*
C4	0.3352 (5)	0.5634 (5)	0.4629 (3)	0.0327 (13)
H4A	0.4273	0.5953	0.4559	0.039*
H4B	0.3124	0.5000	0.4992	0.039*
C5	0.3097 (6)	0.6723 (5)	0.4867 (3)	0.0383 (15)
H5A	0.3181	0.7272	0.4468	0.046*
H5B	0.2206	0.6377	0.5001	0.046*
C6	0.1303 (6)	−0.1879 (6)	−0.1992 (3)	0.0536 (18)
H6A	0.1289	−0.2671	−0.2139	0.080*
H6B	0.1469	−0.1334	−0.2391	0.080*
H6C	0.0472	−0.2053	−0.1825	0.080*
C7	0.3621 (6)	−0.1187 (6)	−0.1575 (3)	0.0509 (17)
H7A	0.4284	−0.0741	−0.1191	0.076*
H7B	0.3885	−0.0749	−0.2011	0.076*
H7C	0.3505	−0.2047	−0.1636	0.076*
C8	0.2499 (6)	0.0073 (5)	−0.1239 (3)	0.0402 (15)
H8A	0.1634	0.0001	−0.1197	0.048*
H8B	0.2860	0.0602	−0.1641	0.048*
C9	0.3351 (6)	0.0743 (5)	−0.0567 (3)	0.0389 (15)
H9A	0.4227	0.0840	−0.0603	0.047*
H9B	0.2997	0.0234	−0.0158	0.047*
C10	0.3409 (6)	0.2042 (6)	−0.0465 (3)	0.0434 (16)
H10A	0.3871	0.2581	−0.0844	0.052*
H10B	0.2525	0.1946	−0.0505	0.052*
C11	0.1445 (6)	0.6791 (6)	0.2703 (3)	0.0394 (15)
H11A	0.2114	0.6593	0.2555	0.059*
H11B	0.0633	0.6017	0.2700	0.059*
H11C	0.1694	0.7183	0.3179	0.059*
C12	0.2544 (6)	0.8844 (6)	0.2121 (3)	0.0472 (17)
H12A	0.2847	0.9338	0.2568	0.071*
H12B	0.2427	0.9359	0.1754	0.071*
H12C	0.3177	0.8579	0.1991	0.071*
C13	0.0264 (6)	0.8086 (6)	0.2393 (3)	0.0386 (15)
H13A	0.0626	0.8698	0.2800	0.046*
H13B	0.0076	0.8515	0.1994	0.046*

C14	−0.0993 (6)	0.6996 (5)	0.2577 (3)	0.0334 (14)
H14A	−0.0909	0.6789	0.3073	0.040*
H14B	−0.1194	0.6243	0.2274	0.040*
C15	−0.2084 (6)	0.7375 (6)	0.2464 (3)	0.0358 (14)
H15A	−0.1832	0.8179	0.2729	0.043*
H15B	−0.2213	0.7506	0.1959	0.043*
N1	0.2463 (4)	0.3797 (4)	0.3702 (2)	0.0313 (11)
H1	0.2109	0.3233	0.4050	0.038*
N2	0.4011 (4)	0.7498 (4)	0.5480 (3)	0.0403 (12)
H2D	0.3817	0.7049	0.5873	0.060*
H2E	0.3938	0.8213	0.5547	0.060*
H2F	0.4828	0.7700	0.5389	0.060*
N3	0.2359 (5)	−0.1227 (4)	−0.1401 (2)	0.0362 (12)
H3	0.2104	−0.1688	−0.1003	0.043*
N4	0.4074 (4)	0.2680 (4)	0.0238 (3)	0.0402 (13)
H4C	0.4890	0.2781	0.0275	0.060*
H4D	0.3640	0.2200	0.0588	0.060*
H4E	0.4091	0.3444	0.0274	0.060*
N5	0.1280 (5)	0.7699 (5)	0.2197 (2)	0.0374 (12)
H5	0.1000	0.7281	0.1758	0.045*
N6	−0.3327 (5)	0.6385 (5)	0.2705 (3)	0.0473 (14)
H6D	−0.3552	0.5642	0.2470	0.071*
H6E	−0.3954	0.6621	0.2615	0.071*
H6F	−0.3225	0.6296	0.3174	0.071*
O1	0.0812 (3)	0.3762 (3)	0.55044 (19)	0.0314 (9)
O2	0.3306 (3)	0.3370 (3)	0.57192 (18)	0.0278 (8)
O3	−0.3799 (3)	−0.0088 (3)	0.61327 (19)	0.0325 (9)
O4	0.2918 (3)	−0.1119 (4)	0.66114 (18)	0.0327 (9)
O5	−0.1423 (3)	0.1722 (3)	0.57991 (17)	0.0229 (8)
O6	−0.3388 (3)	−0.1664 (3)	0.52301 (17)	0.0226 (8)
O7	0.2912 (3)	0.1067 (3)	0.61371 (16)	0.0210 (8)
O8	0.0956 (3)	−0.2327 (3)	0.55729 (17)	0.0235 (8)
O9	0.3267 (3)	−0.0501 (3)	0.52439 (18)	0.0241 (8)
O10	−0.1539 (3)	−0.0427 (3)	0.62667 (17)	0.0220 (8)
O11	0.0655 (3)	−0.0732 (3)	0.64332 (16)	0.0214 (8)
O12	0.0795 (3)	0.1475 (3)	0.59142 (16)	0.0180 (7)
O13	−0.1227 (3)	−0.2032 (3)	0.53428 (16)	0.0180 (7)
O14	0.1072 (3)	−0.0160 (3)	0.50820 (15)	0.0163 (7)
O15	0.0699 (3)	0.8761 (3)	0.03827 (19)	0.0324 (9)
O16	0.3277 (3)	0.8510 (3)	0.04986 (19)	0.0312 (9)
O17	−0.3650 (3)	0.4919 (3)	0.12861 (19)	0.0328 (9)
O18	0.3275 (3)	0.4259 (3)	0.15481 (18)	0.0328 (9)
O19	−0.1398 (3)	0.6720 (3)	0.08191 (17)	0.0236 (8)
O20	−0.3294 (3)	0.3285 (3)	0.03886 (17)	0.0232 (8)
O21	0.3096 (3)	0.6320 (3)	0.10206 (17)	0.0222 (8)
O22	0.1193 (3)	0.2858 (3)	0.05863 (17)	0.0245 (8)
O23	0.3388 (3)	0.4694 (3)	0.01366 (17)	0.0229 (8)
O24	−0.1333 (3)	0.4677 (3)	0.13348 (16)	0.0226 (8)
O25	0.0919 (3)	0.4484 (3)	0.14297 (16)	0.0230 (8)

O26	0.0866 (3)	0.6587 (3)	0.08654 (16)	0.0194 (7)
O27	−0.1086 (3)	0.3007 (3)	0.04267 (16)	0.0194 (7)
O28	0.1101 (3)	0.4891 (3)	0.00524 (15)	0.0176 (7)
O29W	0.1019 (4)	0.5780 (4)	0.6443 (2)	0.0519 (12)
H29B	0.0787	0.6370	0.6219	0.062*
H29A	0.0678	0.5048	0.6159	0.062*
O30W	0.4552 (4)	0.8194 (4)	0.3381 (2)	0.0510 (12)
H30A	0.4373	0.8781	0.3504	0.061*
H30B	0.5336	0.8400	0.3569	0.061*
O31W	0.5050 (4)	0.7341 (5)	0.2138 (2)	0.0691 (16)
H31A	0.4401	0.7063	0.1744	0.083*
H31B	0.4756	0.7602	0.2450	0.083*
O32W	0.3581 (5)	0.6211 (4)	0.6865 (3)	0.0694 (14)
H32A	0.2789	0.6135	0.6890	0.083*
H32B	0.4049	0.6618	0.7262	0.083*
O33W	−0.1878 (5)	0.8894 (4)	−0.1162 (3)	0.0828 (18)
H33A	−0.1447	0.9474	−0.0819	0.099*
H33B	−0.1489	0.8321	−0.1110	0.099*
O34W	0.4372 (7)	0.2430 (6)	0.2017 (4)	0.134 (3)
H34A	0.4070	0.3078	0.1972	0.161*
H34B	0.3874	0.1859	0.1747	0.161*
V1	−0.00384 (8)	0.22701 (8)	0.52518 (4)	0.0204 (2)
V2	0.24366 (8)	0.18796 (8)	0.54459 (4)	0.0200 (2)
V3	−0.27039 (8)	0.00560 (8)	0.56005 (5)	0.0229 (2)
V4	0.22029 (9)	−0.07189 (9)	0.59676 (4)	0.0241 (2)
V5	−0.02534 (8)	−0.03266 (8)	0.58388 (4)	0.0166 (2)
V6	−0.01327 (8)	0.72388 (8)	0.01871 (4)	0.0210 (2)
V7	0.24429 (8)	0.69956 (8)	0.03168 (4)	0.0203 (2)
V8	−0.26351 (8)	0.50339 (8)	0.07083 (5)	0.0236 (2)
V9	0.24551 (9)	0.45527 (9)	0.09123 (5)	0.0242 (2)
V10	−0.01191 (8)	0.47419 (8)	0.08540 (4)	0.0173 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.054 (4)	0.046 (4)	0.028 (3)	0.008 (3)	0.004 (3)	0.007 (3)
C2	0.043 (4)	0.051 (4)	0.058 (4)	0.024 (4)	0.014 (3)	0.000 (3)
C3	0.036 (4)	0.031 (4)	0.052 (4)	0.015 (3)	0.003 (3)	0.012 (3)
C4	0.030 (3)	0.028 (3)	0.042 (4)	0.014 (3)	0.003 (3)	0.004 (3)
C5	0.036 (3)	0.039 (4)	0.047 (4)	0.023 (3)	0.001 (3)	0.004 (3)
C6	0.052 (4)	0.047 (4)	0.033 (4)	−0.001 (3)	−0.002 (3)	0.004 (3)
C7	0.062 (5)	0.049 (4)	0.045 (4)	0.027 (4)	0.014 (3)	0.007 (3)
C8	0.034 (3)	0.034 (4)	0.049 (4)	0.013 (3)	0.001 (3)	0.012 (3)
C9	0.035 (3)	0.036 (4)	0.050 (4)	0.021 (3)	−0.002 (3)	−0.002 (3)
C10	0.045 (4)	0.038 (4)	0.053 (4)	0.026 (3)	−0.006 (3)	0.003 (3)
C11	0.053 (4)	0.046 (4)	0.035 (3)	0.037 (3)	−0.001 (3)	−0.001 (3)
C12	0.043 (4)	0.051 (4)	0.044 (4)	0.020 (4)	−0.003 (3)	0.006 (3)
C13	0.049 (4)	0.034 (4)	0.037 (3)	0.024 (3)	−0.008 (3)	−0.009 (3)

C14	0.046 (4)	0.040 (4)	0.022 (3)	0.027 (3)	−0.003 (3)	−0.001 (3)
C15	0.043 (4)	0.044 (4)	0.028 (3)	0.026 (3)	0.001 (3)	−0.003 (3)
N1	0.032 (3)	0.027 (3)	0.027 (3)	0.007 (2)	0.007 (2)	0.008 (2)
N2	0.028 (3)	0.033 (3)	0.058 (3)	0.013 (2)	0.008 (2)	−0.001 (2)
N3	0.041 (3)	0.033 (3)	0.026 (3)	0.008 (2)	0.006 (2)	0.008 (2)
N4	0.025 (3)	0.031 (3)	0.065 (4)	0.014 (2)	0.004 (2)	0.003 (3)
N5	0.051 (3)	0.045 (3)	0.022 (3)	0.028 (3)	−0.004 (2)	−0.003 (2)
N6	0.051 (3)	0.055 (4)	0.043 (3)	0.029 (3)	0.010 (3)	−0.002 (3)
O1	0.033 (2)	0.021 (2)	0.041 (2)	0.0126 (18)	0.0011 (17)	−0.0058 (17)
O2	0.024 (2)	0.019 (2)	0.033 (2)	0.0046 (17)	−0.0010 (16)	−0.0026 (16)
O3	0.027 (2)	0.039 (2)	0.036 (2)	0.0176 (19)	0.0104 (17)	−0.0018 (18)
O4	0.031 (2)	0.042 (2)	0.030 (2)	0.022 (2)	−0.0005 (17)	0.0059 (18)
O5	0.026 (2)	0.0203 (19)	0.0259 (19)	0.0137 (17)	0.0032 (15)	−0.0038 (15)
O6	0.0183 (18)	0.0210 (19)	0.0268 (19)	0.0071 (16)	0.0043 (15)	0.0004 (15)
O7	0.0192 (18)	0.023 (2)	0.0215 (18)	0.0114 (16)	−0.0040 (14)	−0.0034 (15)
O8	0.031 (2)	0.019 (2)	0.0261 (19)	0.0160 (17)	0.0006 (15)	0.0019 (15)
O9	0.0201 (19)	0.023 (2)	0.032 (2)	0.0131 (17)	0.0004 (15)	−0.0002 (16)
O10	0.0252 (19)	0.022 (2)	0.0208 (18)	0.0128 (17)	0.0034 (15)	0.0016 (15)
O11	0.0257 (19)	0.023 (2)	0.0165 (18)	0.0126 (17)	0.0003 (14)	0.0028 (15)
O12	0.0186 (18)	0.0155 (18)	0.0205 (18)	0.0086 (15)	0.0013 (14)	−0.0017 (14)
O13	0.0164 (18)	0.0148 (18)	0.0210 (18)	0.0055 (15)	0.0024 (14)	0.0025 (14)
O14	0.0178 (18)	0.0140 (17)	0.0174 (17)	0.0074 (15)	0.0022 (13)	−0.0006 (13)
O15	0.032 (2)	0.019 (2)	0.044 (2)	0.0106 (18)	−0.0005 (18)	−0.0064 (17)
O16	0.028 (2)	0.023 (2)	0.037 (2)	0.0078 (17)	−0.0005 (17)	−0.0008 (17)
O17	0.029 (2)	0.037 (2)	0.036 (2)	0.0176 (19)	0.0077 (17)	−0.0020 (18)
O18	0.034 (2)	0.040 (2)	0.030 (2)	0.022 (2)	−0.0027 (17)	0.0022 (18)
O19	0.026 (2)	0.025 (2)	0.0250 (19)	0.0156 (17)	0.0023 (15)	−0.0033 (15)
O20	0.0198 (19)	0.026 (2)	0.0259 (19)	0.0116 (17)	0.0052 (15)	0.0033 (15)
O21	0.0223 (19)	0.023 (2)	0.0219 (19)	0.0121 (17)	−0.0043 (14)	−0.0016 (15)
O22	0.026 (2)	0.021 (2)	0.028 (2)	0.0124 (17)	−0.0002 (15)	0.0024 (16)
O23	0.0235 (19)	0.023 (2)	0.0258 (19)	0.0136 (17)	0.0002 (15)	−0.0011 (15)
O24	0.025 (2)	0.024 (2)	0.0205 (18)	0.0125 (17)	0.0040 (15)	0.0017 (15)
O25	0.028 (2)	0.024 (2)	0.0178 (18)	0.0122 (17)	0.0016 (15)	0.0017 (15)
O26	0.0226 (19)	0.0164 (19)	0.0190 (18)	0.0090 (16)	0.0007 (14)	−0.0035 (14)
O27	0.0187 (18)	0.0156 (18)	0.0223 (18)	0.0066 (15)	0.0010 (14)	0.0009 (14)
O28	0.0197 (18)	0.0160 (18)	0.0162 (17)	0.0076 (15)	0.0011 (14)	−0.0018 (14)
O29W	0.077 (3)	0.033 (3)	0.050 (3)	0.030 (3)	0.000 (2)	0.000 (2)
O30W	0.030 (2)	0.053 (3)	0.069 (3)	0.021 (2)	−0.014 (2)	−0.023 (2)
O31W	0.057 (3)	0.111 (4)	0.053 (3)	0.055 (3)	−0.022 (2)	−0.037 (3)
O32W	0.064 (3)	0.071 (4)	0.080 (4)	0.038 (3)	0.002 (3)	−0.002 (3)
O33W	0.124 (5)	0.042 (3)	0.083 (4)	0.045 (3)	−0.038 (3)	−0.009 (3)
O34W	0.145 (7)	0.109 (6)	0.159 (7)	0.073 (5)	−0.017 (5)	−0.037 (5)
V1	0.0211 (5)	0.0155 (5)	0.0259 (5)	0.0098 (4)	0.0010 (4)	−0.0017 (4)
V2	0.0170 (5)	0.0170 (5)	0.0244 (5)	0.0069 (4)	−0.0016 (4)	−0.0023 (4)
V3	0.0201 (5)	0.0258 (5)	0.0255 (5)	0.0126 (4)	0.0038 (4)	0.0002 (4)
V4	0.0255 (5)	0.0280 (5)	0.0231 (5)	0.0164 (4)	−0.0005 (4)	0.0024 (4)
V5	0.0181 (5)	0.0163 (5)	0.0160 (4)	0.0085 (4)	0.0010 (3)	0.0001 (3)
V6	0.0216 (5)	0.0166 (5)	0.0262 (5)	0.0103 (4)	0.0004 (4)	−0.0007 (4)
V7	0.0183 (5)	0.0183 (5)	0.0233 (5)	0.0078 (4)	−0.0001 (4)	−0.0010 (4)

V8	0.0220 (5)	0.0265 (5)	0.0245 (5)	0.0128 (4)	0.0038 (4)	−0.0007 (4)
V9	0.0252 (5)	0.0276 (5)	0.0242 (5)	0.0164 (4)	−0.0010 (4)	0.0018 (4)
V10	0.0185 (5)	0.0172 (5)	0.0158 (4)	0.0079 (4)	0.0005 (3)	−0.0005 (3)

Geometric parameters (Å, °)

C1—N1	1.489 (6)	V4—O4	1.603 (3)
C1—H1A	0.9600	O5—V1	1.822 (3)
C1—H1B	0.9600	O5—V3	1.845 (3)
C1—H1C	0.9600	O6—V2^{i}	1.822 (3)
C2—N1	1.486 (7)	O6—V3	1.902 (3)
C2—H2A	0.9600	O7—V2	1.810 (3)
C2—H2B	0.9600	O7—V4	1.883 (3)
C2—H2C	0.9600	O8—V1^{i}	1.825 (3)
C3—N1	1.480 (6)	O8—V4	1.873 (3)
C3—C4	1.507 (7)	O9—V4	1.834 (3)
C3—H3A	0.9700	O9—V3^{i}	1.834 (3)
C3—H3B	0.9700	O10—V5	1.693 (3)
C4—C5	1.508 (7)	O10—V3	2.035 (3)
C4—H4A	0.9700	O11—V5	1.690 (3)
C4—H4B	0.9700	O11—V4	2.036 (3)
C5—N2	1.477 (7)	O12—V5	1.893 (3)
C5—H5A	0.9700	O12—V1	1.999 (3)
C5—H5B	0.9700	O12—V2	1.999 (3)
C6—N3	1.491 (7)	O13—V5	1.972 (3)
C6—H6A	0.9600	O13—V1^{i}	2.012 (3)
C6—H6B	0.9600	O13—V2^{i}	2.021 (3)
C6—H6C	0.9600	O14—V5	2.103 (3)
C7—N3	1.494 (7)	O14—V5^{i}	2.111 (3)
C7—H7A	0.9600	O14—V2	2.244 (3)
C7—H7B	0.9600	O14—V1^{i}	2.260 (3)
C7—H7C	0.9600	O14—V3^{i}	2.308 (3)
C8—N3	1.485 (7)	O14—V4	2.315 (3)
C8—C9	1.502 (7)	V6—O15	1.617 (3)
C8—H8A	0.9700	V7—O16	1.605 (3)
C8—H8B	0.9700	V8—O17	1.612 (4)
C9—C10	1.507 (7)	V9—O18	1.602 (3)
C9—H9A	0.9700	O19—V6	1.829 (3)
C9—H9B	0.9700	O19—V8	1.832 (3)
C10—N4	1.479 (7)	O20—V7^{ii}	1.814 (3)
C10—H10A	0.9700	O20—V8	1.907 (3)
C10—H10B	0.9700	O21—V7	1.830 (3)
C11—N5	1.499 (6)	O21—V9	1.860 (3)
C11—H11A	0.9600	O22—V6^{ii}	1.792 (3)
C11—H11B	0.9600	O22—V9	1.909 (3)
C11—H11C	0.9600	O23—V9	1.832 (3)
C12—N5	1.480 (7)	O23—V8^{ii}	1.848 (3)

C12—H12A	0.9600	O24—V10	1.691 (3)
C12—H12B	0.9600	O24—V8	2.032 (3)
C12—H12C	0.9600	O25—V10	1.682 (3)
C13—C14	1.495 (8)	O25—V9	2.050 (3)
C13—N5	1.503 (7)	O26—V10	1.930 (3)
C13—H13A	0.9700	O26—V7	2.018 (3)
C13—H13B	0.9700	O26—V6	2.032 (3)
C14—C15	1.518 (7)	O27—V10	1.948 (3)
C14—H14A	0.9700	O27—V6^{ii}	1.995 (3)
C14—H14B	0.9700	O27—V7^{ii}	2.014 (3)
C15—N6	1.477 (7)	O28—V10	2.085 (3)
C15—H15A	0.9700	O28—V10^{ii}	2.126 (3)
C15—H15B	0.9700	O28—V6^{ii}	2.247 (3)
N1—H1	0.9100	O28—V7	2.260 (3)
N2—H2D	0.8900	O28—V8^{ii}	2.321 (3)
N2—H2E	0.8900	O28—V9	2.322 (3)
N2—H2F	0.8900	O29W—H29B	0.9411
N3—H3	0.9100	O29W—H29A	0.9099
N4—H4C	0.8900	O30W—H30A	0.8405
N4—H4D	0.8900	O30W—H30B	0.8660
N4—H4E	0.8900	O31W—H31A	0.9488
N5—H5	0.9100	O31W—H31B	0.8181
N6—H6D	0.8900	O32W—H32A	0.8804
N6—H6E	0.8900	O32W—H32B	0.8766
N6—H6F	0.8900	O33W—H33A	0.8700
V1—O1	1.612 (3)	O33W—H33B	0.9676
V2—O2	1.622 (3)	O34W—H34A	0.9720
V3—O3	1.614 (3)	O34W—H34B	0.7962
N1—C1—H1A	109.5	V6^{ii}—O28—V8^{ii}	85.28 (11)
N1—C1—H1B	109.5	V7—O28—V8^{ii}	86.66 (11)
H1A—C1—H1B	109.5	V10—O28—V9	88.12 (11)
N1—C1—H1C	109.5	V10^{ii}—O28—V9	170.14 (16)
H1A—C1—H1C	109.5	V6^{ii}—O28—V9	86.37 (11)
H1B—C1—H1C	109.5	V7—O28—V9	84.85 (11)
N1—C2—H2A	109.5	V8^{ii}—O28—V9	83.17 (10)
N1—C2—H2B	109.5	H29B—O29W—H29A	108.4
H2A—C2—H2B	109.5	H30A—O30W—H30B	107.1
N1—C2—H2C	109.5	H31A—O31W—H31B	105.3
H2A—C2—H2C	109.5	H32A—O32W—H32B	107.3
H2B—C2—H2C	109.5	H33A—O33W—H33B	102.4
N1—C3—C4	115.2 (4)	H34A—O34W—H34B	104.1
N1—C3—H3A	108.5	O1—V1—O5	103.12 (17)
C4—C3—H3A	108.5	O1—V1—O8^{i}	102.97 (17)
N1—C3—H3B	108.5	O5—V1—O8^{i}	95.31 (15)
C4—C3—H3B	108.5	O1—V1—O12	100.68 (16)
H3A—C3—H3B	107.5	O5—V1—O12	89.63 (14)

C3—C4—C5	108.5 (4)	O8^{i}—V1—O12	154.03 (14)
C3—C4—H4A	110.0	O1—V1—O13^{i}	100.41 (16)
C5—C4—H4A	110.0	O5—V1—O13^{i}	154.35 (14)
C3—C4—H4B	110.0	O8^{i}—V1—O13^{i}	89.21 (14)
C5—C4—H4B	110.0	O12—V1—O13^{i}	76.03 (13)
H4A—C4—H4B	108.4	O1—V1—O14^{i}	175.06 (15)
N2—C5—C4	112.4 (4)	O5—V1—O14^{i}	79.86 (13)
N2—C5—H5A	109.1	O8^{i}—V1—O14^{i}	80.52 (13)
C4—C5—H5A	109.1	O12—V1—O14^{i}	75.27 (12)
N2—C5—H5B	109.1	O13^{i}—V1—O14^{i}	76.00 (12)
C4—C5—H5B	109.1	O2—V2—O7	101.61 (16)
H5A—C5—H5B	107.9	O2—V2—O6^{i}	103.40 (17)
N3—C6—H6A	109.5	O7—V2—O6^{i}	95.38 (15)
N3—C6—H6B	109.5	O2—V2—O12	99.67 (16)
H6A—C6—H6B	109.5	O7—V2—O12	90.05 (14)
N3—C6—H6C	109.5	O6^{i}—V2—O12	154.66 (14)
H6A—C6—H6C	109.5	O2—V2—O13^{i}	100.90 (15)
H6B—C6—H6C	109.5	O7—V2—O13^{i}	155.12 (14)
N3—C7—H7A	109.5	O6^{i}—V2—O13^{i}	89.56 (14)
N3—C7—H7B	109.5	O12—V2—O13^{i}	75.83 (13)
H7A—C7—H7B	109.5	O2—V2—O14	174.78 (15)
N3—C7—H7C	109.5	O7—V2—O14	80.76 (13)
H7A—C7—H7C	109.5	O6^{i}—V2—O14	80.89 (13)
H7B—C7—H7C	109.5	O12—V2—O14	75.58 (12)
N3—C8—C9	115.0 (4)	O13^{i}—V2—O14	75.97 (12)
N3—C8—H8A	108.5	O3—V3—O9^{i}	103.59 (16)
C9—C8—H8A	108.5	O3—V3—O5	102.92 (17)
N3—C8—H8B	108.5	O9^{i}—V3—O5	91.38 (15)
C9—C8—H8B	108.5	O3—V3—O6	100.78 (17)
H8A—C8—H8B	107.5	O9^{i}—V3—O6	90.14 (15)
C8—C9—C10	109.6 (5)	O5—V3—O6	155.18 (14)
C8—C9—H9A	109.7	O3—V3—O10	99.79 (16)
C10—C9—H9A	109.7	O9^{i}—V3—O10	156.55 (14)
C8—C9—H9B	109.7	O5—V3—O10	85.03 (14)
C10—C9—H9B	109.7	O6—V3—O10	83.79 (14)
H9A—C9—H9B	108.2	O3—V3—O14^{i}	174.52 (15)
N4—C10—C9	112.5 (5)	O9^{i}—V3—O14^{i}	81.70 (13)
N4—C10—H10A	109.1	O5—V3—O14^{i}	78.12 (13)
C9—C10—H10A	109.1	O6—V3—O14^{i}	77.59 (13)
N4—C10—H10B	109.1	O10—V3—O14^{i}	74.88 (12)
C9—C10—H10B	109.1	O4—V4—O9	101.91 (17)
H10A—C10—H10B	107.8	O4—V4—O8	101.43 (17)
N5—C11—H11A	109.5	O9—V4—O8	91.83 (15)

N5—C11—H11B	109.5	O4—V4—O7	102.55 (17)
H11A—C11—H11B	109.5	O9—V4—O7	91.52 (15)
N5—C11—H11C	109.5	O8—V4—O7	154.52 (14)
H11A—C11—H11C	109.5	O4—V4—O11	102.08 (16)
H11B—C11—H11C	109.5	O9—V4—O11	156.01 (14)
N5—C12—H12A	109.5	O8—V4—O11	83.94 (14)
N5—C12—H12B	109.5	O7—V4—O11	82.79 (14)
H12A—C12—H12B	109.5	O4—V4—O14	176.56 (15)
N5—C12—H12C	109.5	O9—V4—O14	81.53 (12)
H12A—C12—H12C	109.5	O8—V4—O14	78.11 (12)
H12B—C12—H12C	109.5	O7—V4—O14	77.43 (12)
C14—C13—N5	114.3 (5)	O11—V4—O14	74.49 (12)
C14—C13—H13A	108.7	O11—V5—O10	106.42 (15)
N5—C13—H13A	108.7	O11—V5—O12	98.35 (15)
C14—C13—H13B	108.7	O10—V5—O12	98.86 (15)
N5—C13—H13B	108.7	O11—V5—O13	96.20 (15)
H13A—C13—H13B	107.6	O10—V5—O13	94.96 (15)
C13—C14—C15	109.1 (5)	O12—V5—O13	156.18 (14)
C13—C14—H14A	109.9	O11—V5—O14	87.61 (14)
C15—C14—H14A	109.9	O10—V5—O14	165.73 (14)
C13—C14—H14B	109.9	O12—V5—O14	81.28 (13)
C15—C14—H14B	109.9	O13—V5—O14	80.60 (13)
H14A—C14—H14B	108.3	O11—V5—O14^{i}	165.84 (14)
N6—C15—C14	111.7 (5)	O10—V5—O14^{i}	87.58 (14)
N6—C15—H15A	109.3	O12—V5—O14^{i}	81.15 (13)
C14—C15—H15A	109.3	O13—V5—O14^{i}	80.15 (12)
N6—C15—H15B	109.3	O14—V5—O14^{i}	78.32 (13)
C14—C15—H15B	109.3	O15—V6—O22^{ii}	103.92 (17)
H15A—C15—H15B	107.9	O15—V6—O19	102.71 (17)
C3—N1—C2	112.8 (4)	O22^{ii}—V6—O19	95.81 (15)
C3—N1—C1	110.3 (4)	O15—V6—O27^{ii}	99.87 (16)
C2—N1—C1	110.2 (4)	O22^{ii}—V6—O27^{ii}	91.11 (14)
C3—N1—H1	107.8	O19—V6—O27^{ii}	153.99 (14)
C2—N1—H1	107.8	O15—V6—O26	99.51 (16)
C1—N1—H1	107.8	O22^{ii}—V6—O26	154.88 (14)
C5—N2—H2D	109.5	O19—V6—O26	87.72 (14)
C5—N2—H2E	109.5	O27^{ii}—V6—O26	75.91 (13)
H2D—N2—H2E	109.5	O15—V6—O28^{ii}	174.18 (15)
C5—N2—H2F	109.5	O22^{ii}—V6—O28^{ii}	80.73 (13)
H2D—N2—H2F	109.5	O19—V6—O28^{ii}	80.07 (13)
H2E—N2—H2F	109.5	O27^{ii}—V6—O28^{ii}	76.34 (12)
C8—N3—C6	109.5 (5)	O26—V6—O28^{ii}	75.38 (12)
C8—N3—C7	112.2 (5)	O15—V6—V7	89.80 (13)
C6—N3—C7	111.6 (5)	O22^{ii}—V6—V7	130.60 (11)
C8—N3—H3	107.8	O19—V6—V7	127.54 (11)

C6—N3—H3	107.8	O27^{ii}—V6—V7	39.52 (9)
C7—N3—H3	107.8	O26—V6—V7	39.82 (9)
C10—N4—H4C	109.5	O28^{ii}—V6—V7	84.48 (9)
C10—N4—H4D	109.5	O16—V7—O20^{ii}	103.06 (18)
H4C—N4—H4D	109.5	O16—V7—O21	102.41 (17)
C10—N4—H4E	109.5	O20^{ii}—V7—O21	95.10 (15)
H4C—N4—H4E	109.5	O16—V7—O27^{ii}	99.75 (16)
H4D—N4—H4E	109.5	O20^{ii}—V7—O27^{ii}	89.78 (14)
C12—N5—C11	111.3 (4)	O21—V7—O27^{ii}	155.56 (14)
C12—N5—C13	110.6 (5)	O16—V7—O26	100.63 (16)
C11—N5—C13	113.4 (4)	O20^{ii}—V7—O26	154.04 (14)
C12—N5—H5	107.0	O21—V7—O26	90.03 (14)
C11—N5—H5	107.0	O27^{ii}—V7—O26	75.80 (13)
C13—N5—H5	107.0	O16—V7—O28	174.69 (15)
C15—N6—H6D	109.5	O20^{ii}—V7—O28	80.36 (13)
C15—N6—H6E	109.5	O21—V7—O28	81.17 (13)
H6D—N6—H6E	109.5	O27^{ii}—V7—O28	76.05 (12)
C15—N6—H6F	109.5	O26—V7—O28	75.31 (12)
H6D—N6—H6F	109.5	O16—V7—V6	90.45 (13)
H6E—N6—H6F	109.5	O20^{ii}—V7—V6	128.83 (11)
V1—O5—V3	115.52 (17)	O21—V7—V6	130.18 (11)
V2^{i}—O6—V3	113.97 (17)	O27^{ii}—V7—V6	39.07 (9)
V2—O7—V4	114.64 (16)	O26—V7—V6	40.16 (9)
V1^{i}—O8—V4	114.51 (17)	O28—V7—V6	84.24 (9)
V4—O9—V3^{i}	113.57 (16)	O17—V8—O19	103.14 (17)
V5—O10—V3	109.96 (16)	O17—V8—O23^{ii}	103.42 (17)
V5—O11—V4	110.27 (16)	O19—V8—O23^{ii}	92.55 (15)
V5—O12—V1	108.38 (15)	O17—V8—O20	101.36 (17)
V5—O12—V2	107.56 (15)	O19—V8—O20	154.51 (14)
V1—O12—V2	101.07 (14)	O23^{ii}—V8—O20	88.51 (14)
V5—O13—V1^{i}	106.68 (15)	O17—V8—O24	100.17 (16)
V5—O13—V2^{i}	106.75 (14)	O19—V8—O24	85.36 (14)
V1^{i}—O13—V2^{i}	99.88 (14)	O23^{ii}—V8—O24	156.17 (14)
V5—O14—V5^{i}	101.68 (13)	O20—V8—O24	83.53 (14)
V5—O14—V2	92.45 (12)	O17—V8—O28^{ii}	174.91 (15)
V5^{i}—O14—V2	94.71 (12)	O19—V8—O28^{ii}	78.03 (13)
V5—O14—V1^{i}	94.12 (12)	O23^{ii}—V8—O28^{ii}	81.41 (13)
V5^{i}—O14—V1^{i}	92.41 (12)	O20—V8—O28^{ii}	76.95 (13)
V2—O14—V1^{i}	169.15 (15)	O24—V8—O28^{ii}	74.92 (12)
V5—O14—V3^{i}	170.82 (15)	O18—V9—O23	103.17 (17)
V5^{i}—O14—V3^{i}	87.50 (11)	O18—V9—O21	102.75 (17)
V2—O14—V3^{i}	86.63 (11)	O23—V9—O21	92.49 (15)
V1^{i}—O14—V3^{i}	85.51 (11)	O18—V9—O22	101.19 (17)

V5—O14—V4	87.64 (11)	O23—V9—O22	90.76 (15)
V5^{i}—O14—V4	170.60 (15)	O21—V9—O22	154.41 (14)
V2—O14—V4	85.99 (11)	O18—V9—O25	101.39 (16)
V1^{i}—O14—V4	85.66 (11)	O23—V9—O25	155.36 (14)
V3^{i}—O14—V4	83.18 (10)	O21—V9—O25	84.10 (14)
V6—O19—V8	115.41 (17)	O22—V9—O25	82.44 (14)
V7^{ii}—O20—V8	115.26 (18)	O18—V9—O28	174.72 (16)
V7—O21—V9	113.80 (16)	O23—V9—O28	81.70 (12)
V6^{ii}—O22—V9	115.30 (17)	O21—V9—O28	78.89 (13)
V9—O23—V8^{ii}	113.72 (16)	O22—V9—O28	76.49 (12)
V10—O24—V8	110.52 (16)	O25—V9—O28	73.69 (12)
V10—O25—V9	110.27 (16)	O25—V10—O24	106.30 (16)
V10—O26—V7	106.79 (15)	O25—V10—O26	97.37 (15)
V10—O26—V6	107.81 (15)	O24—V10—O26	96.91 (15)
V7—O26—V6	100.02 (14)	O25—V10—O27	97.73 (15)
V10—O27—V6^{ii}	106.02 (15)	O24—V10—O27	96.00 (15)
V10—O27—V7^{ii}	107.35 (15)	O26—V10—O27	156.51 (13)
V6^{ii}—O27—V7^{ii}	101.41 (14)	O25—V10—O28	87.90 (14)
V10—O28—V10^{ii}	101.68 (13)	O24—V10—O28	165.79 (14)
V10—O28—V6^{ii}	93.19 (13)	O26—V10—O28	81.38 (13)
V10^{ii}—O28—V6^{ii}	94.09 (12)	O27—V10—O28	81.30 (13)
V10—O28—V7	93.59 (12)	O25—V10—O28^{ii}	166.22 (14)
V10^{ii}—O28—V7	93.37 (12)	O24—V10—O28^{ii}	87.48 (14)
V6^{ii}—O28—V7	168.71 (15)	O26—V10—O28^{ii}	80.38 (13)
V10—O28—V8^{ii}	171.23 (15)	O27—V10—O28^{ii}	80.66 (13)
V10^{ii}—O28—V8^{ii}	87.05 (11)	O28—V10—O28^{ii}	78.32 (13)
N1—C3—C4—C5	−168.4 (5)	V10—O26—V6—V7	−111.39 (19)
C3—C4—C5—N2	−171.0 (5)	V9—O21—V7—O16	−173.84 (19)
N3—C8—C9—C10	−179.9 (5)	V9—O21—V7—O20^{ii}	−69.24 (19)
C8—C9—C10—N4	171.8 (5)	V9—O21—V7—O27^{ii}	31.5 (4)
N5—C13—C14—C15	−156.9 (4)	V9—O21—V7—O26	85.27 (18)
C13—C14—C15—N6	−174.4 (4)	V9—O21—V7—O28	10.15 (16)
C4—C3—N1—C2	−58.7 (6)	V9—O21—V7—V6	84.83 (19)
C4—C3—N1—C1	177.6 (5)	V10—O26—V7—O16	−169.93 (16)
C9—C8—N3—C6	169.2 (5)	V6—O26—V7—O16	77.88 (17)
C9—C8—N3—C7	−66.2 (6)	V10—O26—V7—O20^{ii}	34.5 (4)
C14—C13—N5—C12	−172.2 (5)	V6—O26—V7—O20^{ii}	−77.7 (3)
C14—C13—N5—C11	−46.3 (6)	V10—O26—V7—O21	−67.29 (16)
V3—O5—V1—O1	175.06 (18)	V6—O26—V7—O21	−179.48 (14)
V3—O5—V1—O8^{i}	70.40 (19)	V10—O26—V7—O27^{ii}	92.58 (16)
V3—O5—V1—O12	−84.06 (18)	V6—O26—V7—O27^{ii}	−19.61 (12)
V3—O5—V1—O13^{i}	−28.9 (4)	V10—O26—V7—O28	13.57 (13)
V3—O5—V1—O14^{i}	−8.96 (16)	V6—O26—V7—O28	−98.62 (14)
V5—O12—V1—O1	169.40 (17)	V10—O26—V7—V6	112.19 (19)

V2—O12—V1—O1	−77.72 (18)	V10—O28—V7—O20^{ii}	177.09 (14)
V5—O12—V1—O5	66.12 (17)	V10^{ii}—O28—V7—O20^{ii}	−80.97 (13)
V2—O12—V1—O5	179.00 (15)	V6^{ii}—O28—V7—O20^{ii}	50.3 (8)
V5—O12—V1—O8^{i}	−35.3 (4)	V8^{ii}—O28—V7—O20^{ii}	5.88 (12)
V2—O12—V1—O8^{i}	77.6 (3)	V9—O28—V7—O20^{ii}	89.31 (12)
V5—O12—V1—O13^{i}	−92.40 (16)	V10—O28—V7—O21	80.34 (14)
V2—O12—V1—O13^{i}	20.48 (13)	V10^{ii}—O28—V7—O21	−177.73 (14)
V5—O12—V1—O14^{i}	−13.50 (13)	V6^{ii}—O28—V7—O21	−46.5 (8)
V2—O12—V1—O14^{i}	99.39 (14)	V8^{ii}—O28—V7—O21	−90.88 (13)
V4—O7—V2—O2	−174.99 (18)	V9—O28—V7—O21	−7.45 (12)
V4—O7—V2—O6^{i}	−70.09 (19)	V10—O28—V7—O27^{ii}	−90.72 (13)
V4—O7—V2—O12	85.12 (18)	V10^{ii}—O28—V7—O27^{ii}	11.22 (12)
V4—O7—V2—O13^{i}	30.6 (4)	V6^{ii}—O28—V7—O27^{ii}	142.5 (8)
V4—O7—V2—O14	9.74 (16)	V8^{ii}—O28—V7—O27^{ii}	98.06 (12)
V5—O12—V2—O2	−167.99 (16)	V9—O28—V7—O27^{ii}	−178.51 (13)
V1—O12—V2—O2	78.50 (17)	V10—O28—V7—O26	−12.03 (11)
V5—O12—V2—O7	−66.20 (16)	V10^{ii}—O28—V7—O26	89.91 (13)
V1—O12—V2—O7	−179.71 (14)	V6^{ii}—O28—V7—O26	−138.8 (8)
V5—O12—V2—O6^{i}	36.6 (4)	V8^{ii}—O28—V7—O26	176.75 (13)
V1—O12—V2—O6^{i}	−76.9 (3)	V9—O28—V7—O26	−99.82 (12)
V5—O12—V2—O13^{i}	93.10 (16)	V10—O28—V7—V6	−51.88 (9)
V1—O12—V2—O13^{i}	−20.41 (13)	V10^{ii}—O28—V7—V6	50.06 (9)
V5—O12—V2—O14	14.25 (13)	V6^{ii}—O28—V7—V6	−178.7 (8)
V1—O12—V2—O14	−99.27 (14)	V8^{ii}—O28—V7—V6	136.90 (8)
V5—O14—V2—O7	80.25 (13)	V9—O28—V7—V6	−139.67 (8)
V5^{i}—O14—V2—O7	−177.81 (14)	O15—V6—V7—O16	−0.87 (19)
V1^{i}—O14—V2—O7	−47.0 (8)	O22^{ii}—V6—V7—O16	107.4 (2)
V3^{i}—O14—V2—O7	−90.60 (13)	O19—V6—V7—O16	−106.82 (19)
V4—O14—V2—O7	−7.21 (12)	O27^{ii}—V6—V7—O16	105.0 (2)
V5—O14—V2—O6^{i}	177.28 (14)	O26—V6—V7—O16	−106.06 (19)
V5^{i}—O14—V2—O6^{i}	−80.78 (14)	O28^{ii}—V6—V7—O16	−179.80 (15)
V1^{i}—O14—V2—O6^{i}	50.0 (8)	O15—V6—V7—O20^{ii}	−108.1 (2)
V3^{i}—O14—V2—O6^{i}	6.43 (12)	O22^{ii}—V6—V7—O20^{ii}	0.2 (2)
V4—O14—V2—O6^{i}	89.82 (12)	O19—V6—V7—O20^{ii}	145.94 (19)
V5—O14—V2—O12	−12.20 (11)	O27^{ii}—V6—V7—O20^{ii}	−2.2 (2)
V5^{i}—O14—V2—O12	89.74 (13)	O26—V6—V7—O20^{ii}	146.7 (2)
V1^{i}—O14—V2—O12	−139.4 (8)	O28^{ii}—V6—V7—O20^{ii}	72.96 (17)
V3^{i}—O14—V2—O12	176.95 (13)	O15—V6—V7—O21	105.87 (19)
V4—O14—V2—O12	−99.66 (12)	O22^{ii}—V6—V7—O21	−145.84 (19)
V5—O14—V2—O13^{i}	−90.88 (13)	O19—V6—V7—O21	−0.08 (19)
V5^{i}—O14—V2—O13^{i}	11.06 (12)	O27^{ii}—V6—V7—O21	−148.2 (2)

V1^{i}—O14—V2—O13^{i}	141.9 (8)	O26—V6—V7—O21	0.68 (19)
V3^{i}—O14—V2—O13^{i}	98.27 (12)	O28^{ii}—V6—V7—O21	−73.06 (16)
V4—O14—V2—O13^{i}	−178.34 (13)	O15—V6—V7—O27^{ii}	−105.9 (2)
V1—O5—V3—O3	−176.69 (19)	O22^{ii}—V6—V7—O27^{ii}	2.4 (2)
V1—O5—V3—O9^{i}	−72.40 (19)	O19—V6—V7—O27^{ii}	148.2 (2)
V1—O5—V3—O6	20.9 (4)	O26—V6—V7—O27^{ii}	148.9 (2)
V1—O5—V3—O10	84.38 (18)	O28^{ii}—V6—V7—O27^{ii}	75.19 (17)
V1—O5—V3—O14^{i}	8.82 (16)	O15—V6—V7—O26	105.19 (19)
V2^{i}—O6—V3—O3	176.95 (18)	O22^{ii}—V6—V7—O26	−146.5 (2)
V2^{i}—O6—V3—O9^{i}	73.09 (19)	O19—V6—V7—O26	−0.76 (19)
V2^{i}—O6—V3—O5	−20.5 (4)	O27^{ii}—V6—V7—O26	−148.9 (2)
V2^{i}—O6—V3—O10	−84.22 (18)	O28^{ii}—V6—V7—O26	−73.73 (16)
V2^{i}—O6—V3—O14^{i}	−8.39 (15)	O15—V6—V7—O28	179.19 (16)
V5—O10—V3—O3	−178.89 (19)	O22^{ii}—V6—V7—O28	−72.52 (17)
V5—O10—V3—O9^{i}	5.4 (4)	O19—V6—V7—O28	73.24 (16)
V5—O10—V3—O5	−76.61 (18)	O27^{ii}—V6—V7—O28	−74.93 (16)
V5—O10—V3—O6	81.19 (18)	O26—V6—V7—O28	73.99 (16)
V5—O10—V3—O14^{i}	2.41 (15)	O28^{ii}—V6—V7—O28	0.26 (15)
V3^{i}—O9—V4—O4	178.96 (19)	V6—O19—V8—O17	−175.33 (18)
V3^{i}—O9—V4—O8	76.87 (19)	V6—O19—V8—O23^{ii}	−70.92 (19)
V3^{i}—O9—V4—O7	−77.87 (18)	V6—O19—V8—O20	21.0 (4)
V3^{i}—O9—V4—O11	−2.3 (5)	V6—O19—V8—O24	85.29 (18)
V3^{i}—O9—V4—O14	−0.82 (16)	V6—O19—V8—O28^{ii}	9.74 (16)
V1^{i}—O8—V4—O4	−173.82 (19)	V7^{ii}—O20—V8—O17	177.13 (18)
V1^{i}—O8—V4—O9	−71.28 (19)	V7^{ii}—O20—V8—O19	−19.0 (4)
V1^{i}—O8—V4—O7	26.1 (4)	V7^{ii}—O20—V8—O23^{ii}	73.74 (19)
V1^{i}—O8—V4—O11	85.04 (18)	V7^{ii}—O20—V8—O24	−83.76 (18)
V1^{i}—O8—V4—O14	9.66 (16)	V7^{ii}—O20—V8—O28^{ii}	−7.79 (16)
V2—O7—V4—O4	173.98 (19)	V10—O24—V8—O17	−179.79 (19)
V2—O7—V4—O9	71.43 (19)	V10—O24—V8—O19	−77.24 (19)
V2—O7—V4—O8	−26.0 (4)	V10—O24—V8—O23^{ii}	8.5 (4)
V2—O7—V4—O11	−85.19 (18)	V10—O24—V8—O20	79.78 (18)
V2—O7—V4—O14	−9.55 (16)	V10—O24—V8—O28^{ii}	1.59 (15)
V5—O11—V4—O4	179.90 (19)	V8^{ii}—O23—V9—O18	177.35 (19)
V5—O11—V4—O9	1.2 (4)	V8^{ii}—O23—V9—O21	−78.94 (19)
V5—O11—V4—O8	−79.66 (18)	V8^{ii}—O23—V9—O22	75.68 (18)
V5—O11—V4—O7	78.54 (18)	V8^{ii}—O23—V9—O25	2.3 (5)
V5—O11—V4—O14	−0.36 (15)	V8^{ii}—O23—V9—O28	−0.55 (16)
V5—O14—V4—O9	−179.10 (14)	V7—O21—V9—O18	175.18 (19)
V2—O14—V4—O9	−86.47 (13)	V7—O21—V9—O23	71.09 (19)
V1^{i}—O14—V4—O9	86.59 (13)	V7—O21—V9—O22	−25.9 (4)
V3^{i}—O14—V4—O9	0.60 (12)	V7—O21—V9—O25	−84.44 (18)

V5—O14—V4—O8	87.21 (14)	V7—O21—V9—O28	−9.95 (16)
V2—O14—V4—O8	179.84 (14)	V6^{ii}—O22—V9—O18	−175.5 (2)
V1^{i}—O14—V4—O8	−7.10 (12)	V6^{ii}—O22—V9—O23	−71.9 (2)
V3^{i}—O14—V4—O8	−93.09 (13)	V6^{ii}—O22—V9—O21	25.4 (4)
V5—O14—V4—O7	−85.62 (13)	V6^{ii}—O22—V9—O25	84.29 (19)
V2—O14—V4—O7	7.00 (12)	V6^{ii}—O22—V9—O28	9.32 (16)
V1^{i}—O14—V4—O7	−179.94 (13)	V10—O25—V9—O18	−178.88 (19)
V3^{i}—O14—V4—O7	94.08 (13)	V10—O25—V9—O23	−3.8 (4)
V5—O14—V4—O11	0.27 (11)	V10—O25—V9—O21	79.26 (18)
V2—O14—V4—O11	92.90 (13)	V10—O25—V9—O22	−78.92 (18)
V1^{i}—O14—V4—O11	−94.04 (13)	V10—O25—V9—O28	−0.85 (15)
V3^{i}—O14—V4—O11	179.98 (13)	V10—O28—V9—O23	179.39 (14)
V4—O11—V5—O10	177.70 (16)	V6^{ii}—O28—V9—O23	86.08 (13)
V4—O11—V5—O12	−80.44 (17)	V7—O28—V9—O23	−86.83 (13)
V4—O11—V5—O13	80.66 (17)	V8^{ii}—O28—V9—O23	0.40 (12)
V4—O11—V5—O14	0.38 (16)	V10—O28—V9—O21	−86.40 (14)
V4—O11—V5—O14^{i}	6.5 (7)	V6^{ii}—O28—V9—O21	−179.71 (14)
V3—O10—V5—O11	179.60 (16)	V7—O28—V9—O21	7.38 (12)
V3—O10—V5—O12	78.11 (17)	V8^{ii}—O28—V9—O21	94.62 (13)
V3—O10—V5—O13	−82.44 (17)	V10—O28—V9—O22	86.59 (14)
V3—O10—V5—O14	−11.3 (7)	V6^{ii}—O28—V9—O22	−6.72 (12)
V3—O10—V5—O14^{i}	−2.54 (16)	V7—O28—V9—O22	−179.63 (14)
V1—O12—V5—O11	179.85 (15)	V8^{ii}—O28—V9—O22	−92.39 (13)
V2—O12—V5—O11	71.35 (17)	V10—O28—V9—O25	0.65 (11)
V1—O12—V5—O10	−71.96 (17)	V6^{ii}—O28—V9—O25	−92.67 (13)
V2—O12—V5—O10	179.54 (15)	V7—O28—V9—O25	94.42 (13)
V1—O12—V5—O13	52.8 (4)	V8^{ii}—O28—V9—O25	−178.34 (13)
V2—O12—V5—O13	−55.7 (4)	V9—O25—V10—O24	−179.56 (16)
V1—O12—V5—O14	93.59 (15)	V9—O25—V10—O26	−80.11 (17)
V2—O12—V5—O14	−14.91 (14)	V9—O25—V10—O27	81.84 (18)
V1—O12—V5—O14^{i}	14.16 (14)	V9—O25—V10—O28	0.91 (16)
V2—O12—V5—O14^{i}	−94.34 (15)	V9—O25—V10—O28^{ii}	−0.5 (7)
V1^{i}—O13—V5—O11	−73.01 (17)	V8—O24—V10—O25	178.10 (16)
V2^{i}—O13—V5—O11	−179.11 (15)	V8—O24—V10—O26	78.31 (17)
V1^{i}—O13—V5—O10	179.84 (15)	V8—O24—V10—O27	−82.01 (17)
V2^{i}—O13—V5—O10	73.75 (16)	V8—O24—V10—O28	−3.8 (7)
V1^{i}—O13—V5—O12	54.4 (4)	V8—O24—V10—O28^{ii}	−1.68 (16)
V2^{i}—O13—V5—O12	−51.7 (4)	V7—O26—V10—O25	72.32 (17)
V1^{i}—O13—V5—O14	13.52 (13)	V6—O26—V10—O25	179.05 (15)
V2^{i}—O13—V5—O14	−92.58 (15)	V7—O26—V10—O24	179.83 (15)
V1^{i}—O13—V5—O14^{i}	93.17 (15)	V6—O26—V10—O24	−73.45 (17)
V2^{i}—O13—V5—O14^{i}	−12.92 (14)	V7—O26—V10—O27	−57.3 (4)
V5^{i}—O14—V5—O11	178.48 (15)	V6—O26—V10—O27	49.4 (4)

V2—O14—V5—O11	−86.20 (14)	V7—O26—V10—O28	−14.41 (14)
V1^{i}—O14—V5—O11	85.16 (14)	V6—O26—V10—O28	92.31 (15)
V4—O14—V5—O11	−0.32 (13)	V7—O26—V10—O28^{ii}	−93.93 (15)
V5^{i}—O14—V5—O10	9.0 (6)	V6—O26—V10—O28^{ii}	12.80 (14)
V2—O14—V5—O10	104.3 (6)	V6^{ii}—O27—V10—O25	−71.81 (17)
V1^{i}—O14—V5—O10	−84.3 (6)	V7^{ii}—O27—V10—O25	−179.59 (16)
V4—O14—V5—O10	−169.8 (5)	V6^{ii}—O27—V10—O24	−179.21 (15)
V5^{i}—O14—V5—O12	−82.69 (14)	V7^{ii}—O27—V10—O24	73.01 (17)
V2—O14—V5—O12	12.63 (12)	V6^{ii}—O27—V10—O26	57.8 (4)
V1^{i}—O14—V5—O12	−176.01 (13)	V7^{ii}—O27—V10—O26	−50.0 (4)
V4—O14—V5—O12	98.52 (12)	V6^{ii}—O27—V10—O28	14.86 (13)
V5^{i}—O14—V5—O13	81.79 (14)	V7^{ii}—O27—V10—O28	−92.92 (15)
V2—O14—V5—O13	177.12 (13)	V6^{ii}—O27—V10—O28^{ii}	94.35 (15)
V1^{i}—O14—V5—O13	−11.53 (11)	V7^{ii}—O27—V10—O28^{ii}	−13.43 (14)
V4—O14—V5—O13	−97.00 (12)	V10^{ii}—O28—V10—O25	−179.66 (16)
V5^{i}—O14—V5—O14^{i}	0.0	V6^{ii}—O28—V10—O25	85.50 (14)
V2—O14—V5—O14^{i}	95.33 (14)	V7—O28—V10—O25	−85.47 (14)
V1^{i}—O14—V5—O14^{i}	−93.32 (14)	V9—O28—V10—O25	−0.76 (13)
V4—O14—V5—O14^{i}	−178.79 (17)	V10^{ii}—O28—V10—O24	2.2 (6)
V8—O19—V6—O15	175.22 (18)	V6^{ii}—O28—V10—O24	−92.7 (6)
V8—O19—V6—O22^{ii}	69.5 (2)	V7—O28—V10—O24	96.4 (6)
V8—O19—V6—O27^{ii}	−35.1 (4)	V9—O28—V10—O24	−178.9 (5)
V8—O19—V6—O26	−85.55 (18)	V10^{ii}—O28—V10—O26	−81.88 (14)
V8—O19—V6—O28^{ii}	−9.99 (16)	V6^{ii}—O28—V10—O26	−176.72 (13)
V8—O19—V6—V7	−85.06 (19)	V7—O28—V10—O26	12.31 (12)
V10—O26—V6—O15	170.52 (17)	V9—O28—V10—O26	97.02 (12)
V7—O26—V6—O15	−78.09 (18)	V10^{ii}—O28—V10—O27	82.19 (14)
V10—O26—V6—O22^{ii}	−30.8 (4)	V6^{ii}—O28—V10—O27	−12.65 (11)
V7—O26—V6—O22^{ii}	80.6 (4)	V7—O28—V10—O27	176.38 (13)
V10—O26—V6—O19	68.01 (17)	V9—O28—V10—O27	−98.91 (12)
V7—O26—V6—O19	179.40 (15)	V10^{ii}—O28—V10—O28^{ii}	0.0
V10—O26—V6—O27^{ii}	−91.60 (16)	V6^{ii}—O28—V10—O28^{ii}	−94.84 (14)
V7—O26—V6—O27^{ii}	19.80 (13)	V7—O28—V10—O28^{ii}	94.19 (14)
V10—O26—V6—O28^{ii}	−12.32 (13)	V9—O28—V10—O28^{ii}	178.91 (17)
V7—O26—V6—O28^{ii}	99.07 (14)		

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O13^{i}	0.91	1.79	2.691 (5)	173
N2—H2D···O32W	0.89	2.08	2.968 (7)	172

N2—H2E···O9^{iii}	0.89	2.05	2.873 (5)	153
N2—H2F···O6^{iv}	0.89	1.89	2.772 (6)	173
N3—H3···O27^{v}	0.91	1.87	2.736 (6)	159
N4—H4C···O20^{vi}	0.89	1.89	2.772 (5)	171
N4—H4D···O33W^{ii}	0.89	2.21	3.035 (7)	154
N4—H4E···O23	0.89	1.99	2.820 (5)	156
N5—H5···O26	0.91	1.82	2.709 (5)	166
N6—H6D···O17	0.89	2.34	3.056 (6)	137
N6—H6D···O32W^{vii}	0.89	2.50	3.046 (7)	120
N6—H6E···O31W^{viii}	0.89	1.89	2.745 (6)	160
N6—H6F···O2^{vii}	0.89	2.12	2.958 (6)	156
O29W—H29A···O1	0.91	2.00	2.848 (5)	154
O29W—H29B···O8^{iii}	0.94	1.90	2.790 (5)	156
O30W—H30A···O3^{vii}	0.84	2.06	2.895 (5)	174
O30W—H30B···O7^{ix}	0.87	1.86	2.716 (5)	173
O31W—H31A···O21	0.95	1.83	2.770 (5)	173
O31W—H31B···O30W	0.82	1.94	2.724 (6)	160
O32W—H32A···O29W	0.88	2.00	2.808 (6)	152
O32W—H32B···O34W^{ix}	0.88	2.03	2.873 (8)	160
O33W—H33A···O15^{x}	0.87	1.98	2.787 (6)	153
O33W—H33B···O22^{ii}	0.97	1.84	2.723 (5)	150
O34W—H34A···O18	0.97	2.11	3.055 (7)	163
O34W—H34B···O33W^{ii}	0.80	2.24	2.903 (8)	141

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (iii) *x*, *y*+1, *z*; (iv) *x*+1, *y*+1, *z*; (v) −*x*, −*y*, −*z*; (vi) *x*+1, *y*, *z*; (ii) −*x*, −*y*+1, −*z*; (vii) −*x*, −*y*+1, −*z*+1; (viii) *x*−1, *y*, *z*; (ix) −*x*+1, −*y*+1, −*z*+1; (x) −*x*, −*y*+2, −*z*.

Fig. 1

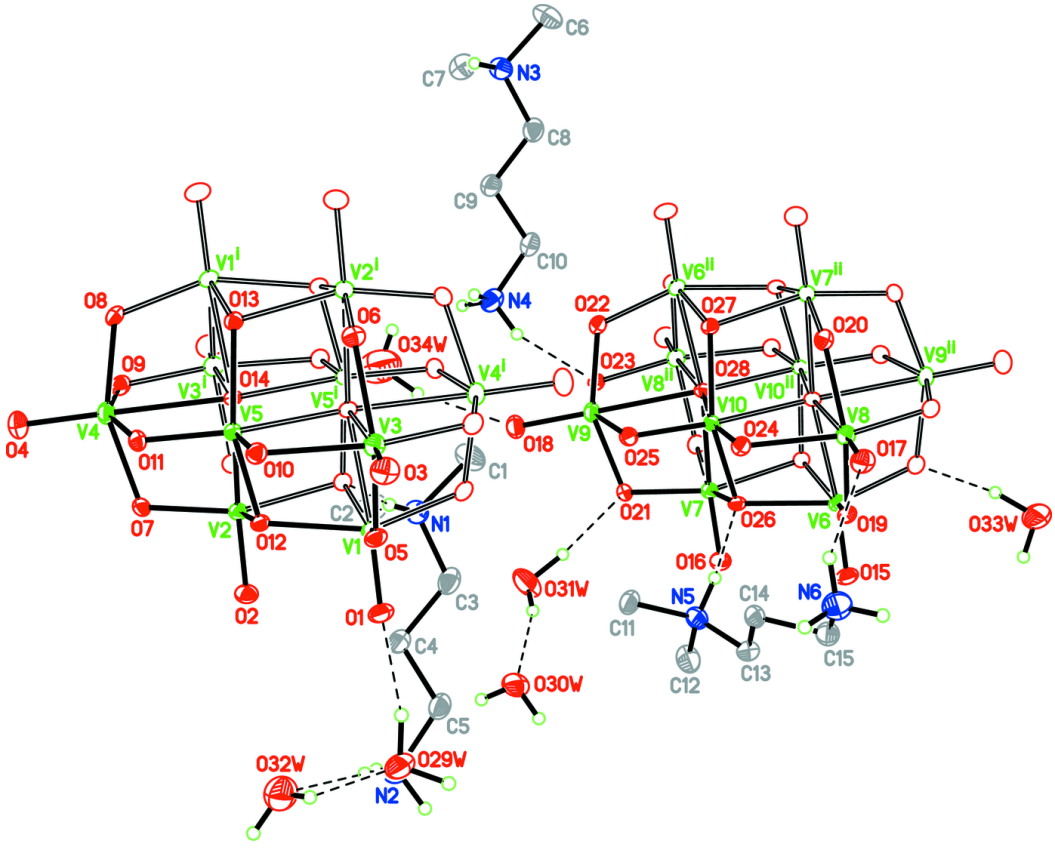
C6
C7
N3
C8
C9
C10
N4
V1I
V2I
O8
O13
O6
O34W
O9
V3I
O14
V5I
V4I
V4
V5
V3
O4
O11
O10
O3
C1
O18
V9
O7
V2
O12
C2
N1
V1
O5
O2
O1
C3
C4
C5
O32W
O29W
N2
O30W
O31W
O22
V6II
V7II
O27
O20
O23
V8II
O28
V10II
V9II
V10
V8
O24
O17
O25
O21
V7
O26
V6
O19
O33W
O16
O15
N5
C14
N6
C11
C12
C13
C15

Fig. 2

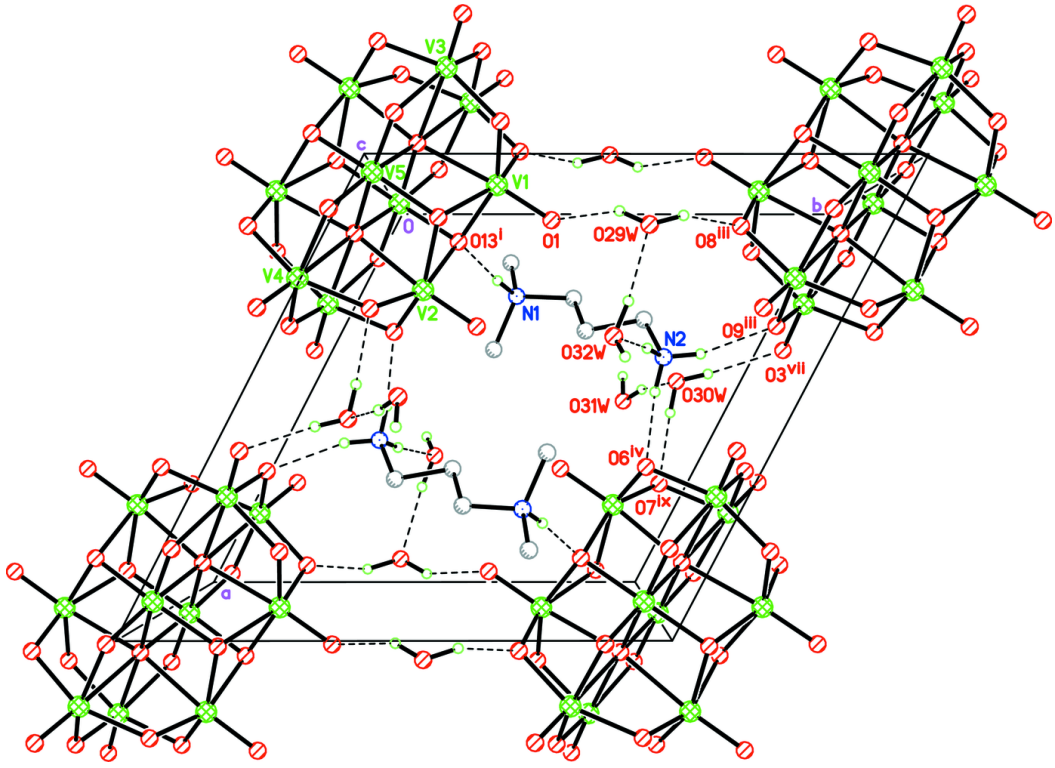
V3
V5
V1
V4
V2
O13^{I}
O1
O29W
O8^{III}
N1
O32W
N2
O9^{III}
O3^{VII}
O31W
O30W
O6^{IV}
O7^{IX}
c
b
a

Fig. 3

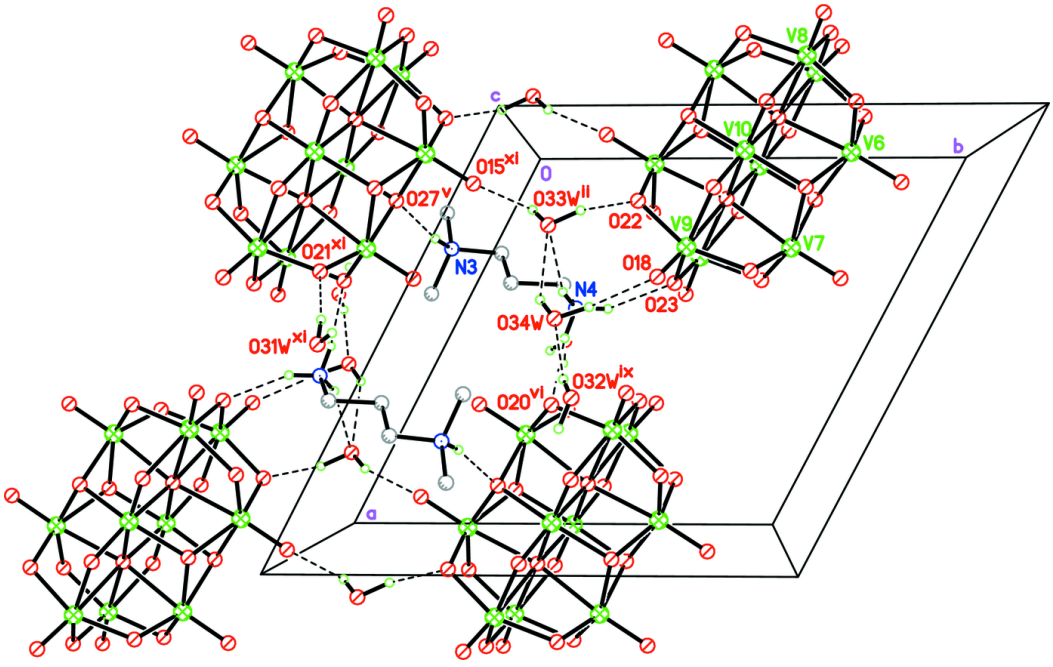
V8
V10
V6
V9
V7
c
b
a
O
N3
N4
O15xi
O27v
O33WII
O22
O18
O23
O21xi
O31Wxi
O34W
O32Wix
O20vi

Fig. 4