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Synthesis and structure of pentakis(2-aminopyridinium) nonavanado(V)tellurate(VI)

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In the title compound, $(C_5H_7N_2)_5[\text{TeV}_9O_{28}]$, the tellurium and vanadium atoms are statistically disordered over two of the ten metal-atom sites in the $[\text{TeV}_9O_{28}]^{5-}$ heteropolyanion. The anions stack along [100] and are extended into a three-dimensional supramolecular network through N-H···O and weak C-H···O hydrogen bonds involving the self-assembled 2-aminopyridinium pentamers, which are linked by C-H··· π and π - π stacking interactions. The most important contributions to the Hirshfeld surface arise from O···H/H···O (54.8%), H···H (17.8%) and C···H/H···C (13.4%) contacts.

1. Chemical context

Tellurium(VI) often occurs as a central octahedral heteroatom in polyoxometalates (POMs) but Te^{VI} is rarely seen in decavanadate (V10) structures: just two vanadotellurates with a decavanadate structure have been reported, *viz*. the monosubstituted tellurium derivative $[H_x \text{TeV}_9 O_{28}]^{(5-x)-}$ described by Konaka *et al.* (2011) and the disubstituted species $[\text{Te}_2 V_9 O_{28}]^{4-}$ reported by our group in the form of its quinolinium salt (Toumi *et al.*, 2013). Moreover, aminopyridine derivatives are commonly used as counter-cations in POMs owing to the easy protonation of their N atoms and their high structural stability (Maalaoui *et al.*, 2013, 2024; Yuan *et al.*, 2009). Here we report the synthesis, structure and Hirshfeld surface analyses of the first unprotonated nonavanado(V) tellurate(VI) cluster, $[\text{TeV}_9 O_{28}]^{5-}$, crystallized as its anhydrous 2-aminopyridinium salt, $(C_5 H_7 N_2)_5 [\text{TeV}_9 O_{28}]$, (I).







2. Structural commentary

The asymmetric unit of (I) consists of one unprotonated $[\text{TeV}_9\text{O}_{28}]^{5-}$ heteropolyanion and five 2-aminopyridinium counter-cations as depicted in Fig. 1. The structure of the heteropolyanion in (I) belongs to the decavanadate structure type (Lee, 2006), but with tellurium replacing one of the vanadium atoms. The Te heteroatom is statistically distributed over the Te1/V9 and Te2/V10 sites in the title compound. This observation is consistent with the structures reported by Konaka *et al.* (2011) in TBA₃[H₂TeV₉O₂₈] and TBA₄



Figure 1

The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius. Non-covalent intermolecular interactions are shown as dotted lines.

 $[HTeV_9O_{28}]$ ·2CH₃CN (TBA = tetrabutyl ammonium). In the $[\text{TeV}_9\text{O}_{28}]^{5-}$ polyanion in (I), the VO₆ octahedra are significantly distorted [range of V–O bond lengths = 1.595(4)– 2.429 (4) Å] whereas the TeO₆ substituted octahedra [Te/ V-O ranges 1.769(4)-2.063(4)Å] are less distorted in comparison with the VO_6 octahedra. The bond-valence sums (BVS; Brown & Altermatt, 1985) for Te1 and Te2 are +6.33 and +6.39 v.u. (v.u. = valence units), whereas those for the V cations are in the range +5.17 v.u. to +5.26 v.u., which are consistent with the oxidation states of Te (+VI) and V (+V). An examination of the 2-aminopyridinium cations show that the bond distances and angles are in accordance with those in analogous salts such as (C₅H₇N₂)₆[V₁₀O₂₈]·2H₂O, (Yuan et al., 2009), $(C_5H_7N_2)_2$ [ReVW₄O₁₉]·7H₂O (Maaloui *et al.*, 2013) and $(C_5H_7N_2)_5[PV_2W_{10}O_{40}] \cdot 0.5(C_5H_5N) \cdot 2H_2O$ (Maaloui et al., 2024).

3. Supramolecular features

In the extended structure, all the hydrogen-bond donors are provided by the five 2-aminopyridinium cations as the poly-



Figure 2

The crystal packing of (I) with $N-H\cdots O$ and weak $C-H\cdots O$ interactions forming a three-dimensional supramolecular network. H atoms not involved in hydrogen bonding scheme are omitted

Table 1Hydrogen-bond geometry (Å, $^{\circ}$).

$D - H \cdot \cdot \cdot A$	$D-{\rm H}$	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdots A$
$N1-H1\cdots O6^{i}$	0.86	2.57	3.426 (8)	172
$N2-H2A\cdotsO1^{i}$	0.86	2.26	3.105 (8)	167
$N2-H2B\cdots O3^{ii}$	0.86	2.50	3.006 (7)	118
$N2-H2B\cdotsO10^{ii}$	0.86	2.28	3.121 (8)	165
$C4-H4\cdots O3E$	0.93	2.44	2.995 (8)	119
$C4-H4\cdots O8E^{iii}$	0.93	2.26	3.073 (8)	146
C5−H5···O9 ⁱⁱⁱ	0.93	2.24	3.136 (8)	161
$N3-H3A\cdotsO12^{iv}$	0.86	2.54	3.397 (7)	175
$N4-H4A\cdots O7^{v}$	0.86	2.05	2.896 (7)	168
$N4-H4B\cdotsO16^{iv}$	0.86	2.19	2.998 (7)	156
$C7-H7\cdots O18^{v}$	0.93	2.57	3.495 (8)	171
$C9-H9\cdots O5^{i}$	0.93	1.86	2.760 (7)	161
$N5-H5A\cdotsO10^{ii}$	0.86	2.61	3.404 (8)	154
N6-H6 A ···O1 E ^{vi}	0.86	2.14	2.922 (8)	151
$N6-H6B\cdots O7E^{ii}$	0.86	2.05	2.900 (8)	171
$C12-H12\cdots O1E^{vi}$	0.93	2.63	3.312 (9)	130
$C14 - H14 \cdots O8^{iv}$	0.93	1.78	2.703 (7)	174
$C14 - H14 \cdots O17^{iv}$	0.93	2.62	3.146 (8)	117
$N7 - H7A \cdots O15^{vi}$	0.86	2.48	3.308 (8)	161
N8-H8 A ···O3 E ^{vii}	0.86	2.12	2.966 (7)	169
$N8 - H8B \cdot \cdot \cdot O14^{vi}$	0.86	2.18	2.963 (7)	152
C19-H19···O13 ⁱⁱ	0.93	1.88	2.788 (7)	165
$C20-H20\cdots O18^{ii}$	0.93	2.43	3.202 (8)	140
N9-H9 A ···O5 E	0.86	2.46	3.244 (7)	151
N10−H10A···O3	0.86	2.30	3.098 (8)	155
$N10-H10B\cdotsO1^{viii}$	0.86	2.65	3.294 (8)	132
$N10-H10B\cdots O2^{vm}$	0.86	2.34	3.169 (8)	162
$C22 - H22 \cdots O2E^{viii}$	0.93	2.29	3.189 (8)	164
$C24 - H24 \cdots O4E^{ix}$	0.93	2.35	2.929 (7)	120
$C24 - H24 \cdots O6E^{ix}$	0.93	2.61	3.153 (7)	118
$C24-H24\cdots O11^{x}$	0.93	2.48	3.003 (7)	116
$C10-H10\cdots Cg1$	0.93	3.07	3.902	151
$C18-H18\cdots Cg5^{iv}$	0.93	2.66	3.450	143

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

anion is unprotonated. Each cation donates hydrogen bonds to the terminal and bridging O atoms of the polyanions stacked along [100] at z = 1/4 and 3/4 by means of N-H···O and weak C-H···O interactions, giving rise to a threedimensional supramolecular network (Fig. 2 and Table 1). Furthermore, the 2-aminopyridinium moieties are themselves





The self-assembled 2-aminopyridinium pentamer featuring weak C-H··· π and π - π stacking interactions (depicted by dashed lines). Other H atoms omitted. Symmetry codes: (iv): $x, \frac{1}{2} - y, \frac{1}{2} + z$; (viii): 1 + x, y, z.

connected by weak $C-H\cdots\pi$ [C10-H10 \cdots Cg1 = 3.066 Å, C18-H18 \cdots Cg5^{iv} = 2.659 Å; symmetry code: (iv) $x, \frac{1}{2} - y, \frac{1}{2} + z$; Table 1] and $\pi-\pi$ stacking interactions between the *R*2/ *R*4 and *R*4/*R*3 pyridyl rings [*R*1 = N1/C1-C5 (centroid *C*g1), *R*2 = N3/C6-C10 (centroid *C*g2), *R*3 = N5/C11-C15 (centroid *C*g3), *R*4 = N7/C16-C20 (centroid *C*g4), R5 = N9/C21-C25 (centroid *C*g5)] stacked in parallel displaced face-to-face arrangements with centroid-centroid distances of 3.724 (2) and 3.829 (2) Å, respectively (Fig. 3), within the accepted rangesfor C-H $\cdots\pi$ and $\pi-\pi$ stacking interactions (Janiak (2000).

4. Hirshfeld surface analysis

Fig. 4(*a*) illustrates the Hirshfeld surface of (I) mapped over d_{norm} with red spots corresponding to short inter-contacts. The

red, triangular concave regions in the Hirshfeld surface mapped with shape index [Fig. 4(*b*)], confirm the existence of the π - π stacking interactions mentioned above. The fingerprint plots (Fig. 5) indicate that the major contact contributions to the crystal structure are from O···H/H···O (54.8%), H···H (17.8%) and C···H/H···C (13.4%) whereas the contributions of the remaining contacts [N···H/H···N (4.7%), O···C/C···O (2.6%), C···C (2.3%), O···O (1.6%)] are very small. The characteristic spikes in the O···H/H···O plot [Fig. 5(*a*)] indicate the existence of the N-H···O and C-H···O hydrogen bonds (Table 1).

5. Database survey

Related vanadotellurates with the decavanadate structure type include $TBA_4[HTeV_9O_{28}]\cdot 2CH_3CN$ and $TBA_3-[H_2TeV_9O_{28}]$ (TBA = tetra-*n*-butylammonium) (Konaka *et al.*,





The Hirshfeld surface mapped over (a) d_{norm} and (b) shape-index. N-H···O and C-H···O hydrogen bonds from neighbouring organic cations are represented by green dotted lines.



Figure 5

Fingerprint plots showing the major contacts contributions of (a) $H \cdots O/O \cdots H$, (b) $H \cdots H$ and (c) $C \cdots H/H \cdots C$.

2011) and $(C_9H_8N)_4[Te_2V_8O_{28}]\cdot 8H_2O$ (Toumi *et al.*, 2013). Related nonavanadoplatinate(IV) clusters include Na₉[H₂PtV₉O₂₈][H₃PtV₉O₂₈]·40H₂O (Joo *et al.*, 2015), Na₅[H₂PtV₉O₂₈]·21H₂O (Lee *et al.*, 2008), (CH₆N₃)₅-[H₂PtV₉O₂₈] (Joo *et al.*, 2011) and K₅[H₂PtV₉O₂₈]·9H₂O (Joo & Lee, 2015). For the related structures of aminopyridinium containing polyoxometalates (C₅H₇N₂)₆[V₁₀O₂₈]·2H₂O, see: Yuan *et al.* (2009); (C₅H₇N₂)₂[ReVW₄O₁₉]·7H₂O, see: Maaloui *et al.* (2013) and (C₅H₇N₂)₅[PV₂W₁₀O₄₀]·0.5(C₅H₅N)·2H₂O, see: Maaloui *et al.* (2024).

6. Synthesis and crystallization

Vanadium(V) oxide (1.26 g, 6.93 mmol), 2-aminopyridine (0.59 g, 6.16 mmol) and telluric acid, $Te(OH)_6$ (0.36 g, 1.55 mmol) were suspended in 50 ml of distilled water. Then the pH value of the mixture was adjusted to 6 with 3 *M* hydrochloric acid (HCl) and stirred for 3 h. After one week, yellow prismatic single crystals were grown by slow evaporation at room temperature.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H-atoms were positioned with idealized geometry and refined using a riding model with C-H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ and N-H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(N)$.

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References

- Blessing, R. H. (1995). Acta Cryst. A51, 33-38.
- Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Brown, I. D. & Altermatt, D. (1985). Acta Cryst. B41, 244-247.
- Enraf-Nonius (1994). *CAD-4 EXPRESS*. Enraf-Nonius, Delft, The Netherlands.
- Farrugia, L. J. (2012). J. Appl. Cryst. 45, 849-854.
- Harms, K. & Wocadlo, S. (1996). XCAD4. University of Marburg, Germany.

Experimental details.

Crystal data	
Chemical formula	$(C_5H_7N_2)_5[TeV_9O_{28}]$
Mr	1509.69
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	11.661 (2), 23.251 (2), 19.602 (3)
β (°)	122.53 (1)
$V(Å^3)$	4481.1 (12)
Z	4
Radiation type	Ag $K\alpha$, $\lambda = 0.56087$ Å
$\mu (\text{mm}^{-1})$	1.31
Crystal size (mm)	$0.25 \times 0.19 \times 0.13$
Data collection	
Diffractometer	Enraf-Nonius CAD-4
Absorption correction	Multi-scan (Blessing, 1995)
T_{\min}, T_{\max}	0.745, 0.807
No. of measured, independent and	25752, 21889, 10265
observed $[I > 2\sigma(I)]$ reflections	
R _{int}	0.048
$(\sin \theta / \lambda)_{\max} (\text{\AA}^{-1})$	0.837
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.076, 0.211, 1.03
No. of reflections	21889
No. of parameters	658
H-atom treatment	H-atom parameters constrained
$\Delta \rho_{\text{max}} \Delta \rho_{\text{min}} (e \text{\AA}^{-3})$	1.191.74

Computer programs: CAD-4 EXPRESS (Enraf–Nonius, 1994), XCAD4 (Harms & Wocadlo, 1996), SHELXS97 (Sheldrick, 2008), SHELXL2018/3 (Sheldrick, 2015), DIAMOND (Brandenburg & Putz, 2005), WinGX publication routines (Farrugia, 2012) and CrystalExplorer (Wolff et al., 2012).

Janiak, J. (2000). J. Chem. Soc. Dalton Trans. pp. 3885-3896.

- Joo, H.-C. & Lee, U. (2015). Acta Cryst. E71, 647-649.
- Joo, H.-C., Park, K.-M. & Lee, U. (2011). Acta Cryst. E67, m1801– m1802.
- Joo, H.-C., Park, K.-M. & Lee, U. (2015). Acta Cryst. E71, 786-790.
- Konaka, S., Ozawa, Y., Shonaka, T., Watanabe, S. & Yagasaki, A. (2011). *Inorg. Chem.* **50**, 6183–6188.
- Lee, U. (2006). Acta Cryst. E62, i176-i178.
- Lee, U., Joo, H.-J., Park, K.-M., Mal, S. S., Kortz, U., Keita, B. & Nadjo, L. (2008). Angew. Chem. Int. Ed. 47, 793–796.
- Maalaoui, A., Guedidi, H., Rzaigui, M. & Akriche, S. (2024). *Energy Fuels*, **38**, 1319–1329.
- Maaloui, A., Toumi, S. A. & Rzaigui, M. (2013). Acta Cryst. E69, m661–m662.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
- Sheldrick, G. M. (2015). Acta Cryst. C71, 3-8.
- Toumi, S., Toumi, S. A. & Rzaigui, M. (2013). Acta Cryst. E69, m595– m596.
- Wolff, S. K., Grimwood, D. J., McKinnon, J. J., Turner, M. J., Jayatilaka, D. & Spackman, M. A. (2012). *CrystalExplorer*. University of Western Australia.
- Yuan, C., Lu, L., Zhu, M., Ma, Q. & Wu, Y. (2009). Acta Cryst. E65, m267–m268.

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Computing details

Pentakis(2-aminopyridinium) nonavanado(V)tellurate(VI)

Crystal data

 $(C_{5}H_{7}N_{2})_{5}[TeV_{9}O_{28}]$ $M_{r} = 1509.69$ Monoclinic, $P2_{1}/c$ a = 11.661 (2) Å b = 23.251 (2) Å c = 19.602 (3) Å $\beta = 122.53$ (1)° V = 4481.1 (12) Å³ Z = 4

Data collection

Enraf–Nonius CAD-4 diffractometer Radiation source: Enraf Nonius FR590 Graphite monochromator non–profiled ω scans Absorption correction: multi-scan (Blessing, 1995) $T_{\min} = 0.745, T_{\max} = 0.807$ 25752 measured reflections

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.076$ $wR(F^2) = 0.211$ S = 1.0321889 reflections 658 parameters 0 restraints Primary atom site location: structure-invariant direct methods F(000) = 2952 $D_x = 2.238 \text{ Mg m}^{-3}$ Ag $K\alpha$ radiation, $\lambda = 0.56087 \text{ Å}$ Cell parameters from 25 reflections $\theta = 9-11^{\circ}$ $\mu = 1.31 \text{ mm}^{-1}$ T = 293 KPrism, yellow $0.25 \times 0.19 \times 0.13 \text{ mm}$

21889 independent reflections 10265 reflections with $I > 2\sigma(I)$ $R_{int} = 0.048$ $\theta_{max} = 28.0^{\circ}, \theta_{min} = 2.1^{\circ}$ $h = -19 \rightarrow 19$ $k = -38 \rightarrow 1$ $l = -21 \rightarrow 32$ 2 standard reflections every 120 min intensity decay: -2%

Secondary atom site location: difference Fourier map Hydrogen site location: difference Fourier map H-atom parameters constrained $w = 1/[\sigma^2(F_o^2) + (0.0646P)^2 + 23.768P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} < 0.001$ $\Delta\rho_{max} = 1.19$ e Å⁻³ $\Delta\rho_{min} = -1.74$ e Å⁻³

Special details

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

	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	Occ. (<1)
V1	-0.04965 (9)	0.09075 (4)	0.20903 (6)	0.02450 (19)	
V2	0.08300 (10)	0.20810 (4)	0.20870 (6)	0.02400 (19)	
V3	0.10819 (10)	0.16241 (4)	0.36755 (6)	0.02479 (19)	
V4	0.22827 (9)	0.04297 (4)	0.35456 (6)	0.02207 (18)	
V5	0.33925 (9)	0.20776 (4)	0.19507 (6)	0.02098 (18)	
V6	0.48299 (9)	0.04162 (4)	0.33892 (6)	0.02189 (18)	
V7	0.45911 (10)	0.09044 (4)	0.18122 (6)	0.02306 (18)	
V8	0.61987 (9)	0.15934 (4)	0.34255 (6)	0.02428 (19)	
Te1	0.20032 (5)	0.08920 (2)	0.19110 (3)	0.02224 (11)	0.5
V9	0.20032 (5)	0.08920 (2)	0.19110 (3)	0.02224 (11)	0.5
Te2	0.36502 (5)	0.16117 (2)	0.35539 (3)	0.01968 (10)	0.5
V10	0.36502 (5)	0.16117 (2)	0.35539 (3)	0.01968 (10)	0.5
O1C	0.1777 (4)	0.12502 (15)	0.2795 (2)	0.0194 (7)	
O2C	0.3881 (4)	0.12507 (15)	0.2679 (2)	0.0184 (7)	
O1E	-0.1978 (4)	0.0632 (2)	0.1558 (3)	0.0345 (10)	
O2E	0.0345 (4)	0.26655 (19)	0.1575 (3)	0.0334 (10)	
O3E	0.0777 (5)	0.18882 (19)	0.4322 (3)	0.0349 (10)	
O4E	0.2796 (4)	-0.01547 (18)	0.4051 (3)	0.0291 (9)	
O5E	0.2880 (4)	0.26650 (18)	0.1446 (3)	0.0303 (9)	
O6E	0.5314 (4)	-0.01715 (18)	0.3887 (3)	0.0323 (9)	
O7E	0.4904 (5)	0.0649 (2)	0.1165 (3)	0.0331 (10)	
O8E	0.7705 (4)	0.1847 (2)	0.3991 (3)	0.0351 (10)	
01	-0.0473 (4)	0.12517 (18)	0.2928 (3)	0.0279 (8)	
O2	-0.0658 (4)	0.16167 (18)	0.1600 (3)	0.0281 (8)	
O3	0.6150 (4)	0.12598 (17)	0.2562 (2)	0.0253 (8)	
O4	0.0704 (4)	0.22175 (17)	0.2957 (3)	0.0274 (8)	
05	0.0520 (4)	0.02864 (17)	0.2764 (2)	0.0252 (8)	
O6	0.1898 (4)	0.09013 (18)	0.4131 (2)	0.0254 (8)	
07	0.3775 (4)	0.16162 (17)	0.1356 (2)	0.0238 (8)	
08	0.5151 (4)	0.22191 (17)	0.2729 (2)	0.0241 (8)	
09	0.6298 (4)	0.08877 (17)	0.3882 (2)	0.0250 (8)	
O10	0.4971 (4)	0.02920 (17)	0.2523 (2)	0.0242 (8)	
011	0.4076 (4)	0.08450 (16)	0.3978 (2)	0.0201 (7)	
O12	0.2858 (4)	0.22228 (15)	0.2773 (2)	0.0207 (7)	
013	0.2804 (4)	0.02707 (16)	0.2701 (2)	0.0196 (7)	
O14	0.1581 (4)	0.16667 (16)	0.1492 (2)	0.0218 (7)	
O15	0.0311 (4)	0.06384 (17)	0.1429 (2)	0.0250 (8)	
016	0.3056 (4)	0.18699 (17)	0.4170 (2)	0.0258 (8)	
O17	0.5353 (4)	0.18601 (17)	0.4046 (2)	0.0244 (8)	

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

O18	0.2607 (4)	0.06431 (17)	0.1304 (2)	0.0259 (8)
N1	-0.0124 (6)	0.0239 (3)	0.5776 (4)	0.0454 (15)
H1	-0.0643	-0.0021	0.5783	0.055*
N2	0.1895 (7)	-0.0268 (3)	0.6727 (4)	0.0466 (16)
H2A	0.1414	-0.0544	0.6739	0.056*
H2B	0.2768	-0.0288	0.7019	0.056*
C1	0.1300 (6)	0.0180 (3)	0.6268 (4)	0.0304 (12)
C2	0.2068 (7)	0.0636 (3)	0.6223 (4)	0.0385 (15)
H2	0.3013	0.0623	0.6537	0.046*
C3	0.1435 (9)	0.1084 (3)	0.5729 (5)	0.0475 (18)
Н3	0.1952	0.1377	0.5701	0.057*
C4	0.0094 (7)	0.1119 (3)	0.5281 (4)	0.0350 (14)
H4	-0.0318	0.1438	0.4950	0.042*
C5	-0.0669(7)	0.0704 (4)	0.5297 (4)	0.0445 (18)
Н5	-0.1611	0.0735	0.4968	0.053*
N3	0.2068 (7)	0.1563 (3)	0.8399 (4)	0.0481 (16)
H3A	0.2313	0.1862	0.8249	0.058*
N4	0.3077 (6)	0.1934 (2)	0.9747 (3)	0.0378 (13)
H4A	0.3277	0.1892	1.0236	0.045*
H4B	0.3303	0.2243	0.9609	0.045*
C6	0.2417 (6)	0.1519 (3)	0.9207 (4)	0.0293 (12)
C7	0.2030 (7)	0.1005 (3)	0.9413 (4)	0.0332 (13)
H7	0.2255	0.0945	0.9940	0.040*
C8	0.1334 (7)	0.0602 (3)	0.8843 (5)	0.0390 (15)
H8	0.1085	0.0266	0.8987	0.047*
C9	0.0989 (6)	0.0666 (2)	0.8084 (4)	0.0284 (11)
Н9	0.0495	0.0379	0.7708	0.034*
C10	0.1343 (8)	0.1138 (3)	0.7853 (5)	0.0451 (17)
H10	0.1096	0.1177	0.7318	0.054*
N5	0.5217 (7)	0.0852 (3)	0.8616 (4)	0.0536 (17)
H5A	0.4945	0.0536	0.8348	0.064*
N6	0.6012 (8)	0.0360 (3)	0.9866 (4)	0.057 (2)
H6A	0.6405	0.0363	1.0384	0.068*
H6B	0.5752	0.0040	0.9606	0.068*
C11	0.5809 (7)	0.0847 (3)	0.9469 (4)	0.0351 (14)
C12	0.6208 (8)	0.1373 (3)	0.9858 (5)	0.0483 (19)
H12	0.6587	0.1394	1.0413	0.058*
C13	0.6045 (9)	0.1859 (3)	0.9429 (5)	0.054 (2)
H13	0.6326	0.2210	0.9697	0.065*
C14	0.5497 (7)	0.1844 (3)	0.8637 (4)	0.0382 (15)
H14	0.5397	0.2183	0.8358	0.046*
C15	0.5084 (8)	0.1344 (3)	0.8233 (5)	0.0474 (18)
H15	0.4699	0.1341	0.7677	0.057*
N7	0.9043 (7)	0.1101 (3)	0.9559 (4)	0.0486 (16)
H7A	0.9288	0.1059	1.0056	0.058*
N8	0.9909 (7)	0.2065 (3)	0.9791 (4)	0.0481 (16)
H8A	1.0041	0.2383	0.9620	0.058*
H8B	1.0190	0.2025	1.0294	0.058*

C16	0.9275 (7)	0.1637 (3)	0.9281 (4)	0.0342 (13)
C17	0.8790 (8)	0.1676 (3)	0.8452 (4)	0.0428 (17)
H17	0.8876	0.2017	0.8236	0.051*
C18	0.8194 (8)	0.1207 (3)	0.7970 (4)	0.0479 (19)
H18	0.7905	0.1229	0.7427	0.057*
C19	0.8012 (7)	0.0718 (3)	0.8253 (4)	0.0350 (14)
H19	0.7582	0.0410	0.7902	0.042*
C20	0.8432 (7)	0.0662 (3)	0.9024 (5)	0.0415 (16)
H20	0.8306	0.0313	0.9206	0.050*
N9	0.5489 (7)	0.2953 (3)	0.1326 (5)	0.058 (2)
H9A	0.5021	0.2796	0.1497	0.070*
N10	0.7082 (7)	0.2180 (3)	0.1817 (4)	0.0533 (17)
H10A	0.6639	0.2009	0.1995	0.064*
H10B	0.7802	0.2024	0.1880	0.064*
C21	0.6657 (6)	0.2680 (3)	0.1446 (4)	0.0305 (12)
C22	0.7364 (7)	0.2980 (3)	0.1143 (5)	0.0393 (15)
H22	0.8148	0.2823	0.1203	0.047*
C23	0.6885 (8)	0.3491 (3)	0.0767 (4)	0.0427 (17)
H23	0.7332	0.3673	0.0552	0.051*
C24	0.5814 (6)	0.3742 (2)	0.0694 (4)	0.0313 (13)
H24	0.5564	0.4109	0.0474	0.038*
C25	0.5100 (7)	0.3475 (3)	0.0933 (5)	0.0457 (18)
H25	0.4301	0.3645	0.0832	0.055*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
V1	0.0177 (4)	0.0258 (5)	0.0284 (5)	-0.0012 (4)	0.0114 (4)	0.0006 (4)
V2	0.0217 (4)	0.0225 (4)	0.0293 (5)	0.0046 (3)	0.0147 (4)	0.0060 (4)
V3	0.0289 (5)	0.0225 (4)	0.0302 (5)	0.0015 (4)	0.0207 (4)	-0.0011 (4)
V4	0.0231 (4)	0.0190 (4)	0.0253 (4)	0.0007 (3)	0.0138 (4)	0.0040 (3)
V5	0.0199 (4)	0.0195 (4)	0.0237 (4)	-0.0004 (3)	0.0119 (4)	0.0035 (3)
V6	0.0195 (4)	0.0201 (4)	0.0254 (4)	0.0027 (3)	0.0116 (4)	0.0030 (3)
V7	0.0223 (4)	0.0253 (4)	0.0239 (4)	0.0002 (4)	0.0141 (4)	-0.0024 (4)
V8	0.0174 (4)	0.0250 (5)	0.0267 (5)	-0.0020 (3)	0.0094 (4)	-0.0028 (4)
Te1	0.0202 (2)	0.0230 (2)	0.0224 (2)	-0.00086 (19)	0.0107 (2)	-0.0001 (2)
V9	0.0202 (2)	0.0230 (2)	0.0224 (2)	-0.00086 (19)	0.0107 (2)	-0.0001 (2)
Te2	0.0208 (2)	0.0180 (2)	0.0200 (2)	0.00005 (18)	0.01080 (18)	0.00028 (18)
V10	0.0208 (2)	0.0180 (2)	0.0200 (2)	0.00005 (18)	0.01080 (18)	0.00028 (18)
O1C	0.0188 (16)	0.0179 (16)	0.0239 (17)	-0.0015 (13)	0.0131 (14)	-0.0024 (14)
O2C	0.0186 (16)	0.0144 (15)	0.0226 (17)	-0.0016 (13)	0.0114 (14)	-0.0013 (13)
O1E	0.0215 (19)	0.042 (3)	0.035 (2)	-0.0065 (18)	0.0117 (18)	-0.002 (2)
O2E	0.029 (2)	0.029 (2)	0.044 (3)	0.0088 (17)	0.021 (2)	0.0153 (19)
O3E	0.047 (3)	0.032 (2)	0.038 (2)	0.001 (2)	0.031 (2)	-0.0063 (19)
O4E	0.032 (2)	0.026 (2)	0.030(2)	0.0061 (17)	0.0166 (18)	0.0089 (17)
O5E	0.030 (2)	0.029 (2)	0.034 (2)	0.0015 (17)	0.0183 (18)	0.0066 (18)
O6E	0.032 (2)	0.027 (2)	0.038 (2)	0.0079 (18)	0.019 (2)	0.0105 (18)
O7E	0.033 (2)	0.042 (3)	0.031 (2)	-0.0019 (19)	0.0212 (19)	-0.0062 (19)

O8E	0.023 (2)	0.037 (2)	0.037 (2)	-0.0078 (18)	0.0104 (18)	-0.008(2)
01	0.028 (2)	0.029 (2)	0.034 (2)	0.0017 (17)	0.0212 (18)	0.0028 (17)
O2	0.0166 (17)	0.028 (2)	0.037 (2)	0.0033 (15)	0.0122 (16)	0.0063 (18)
03	0.0210 (18)	0.0259 (19)	0.030 (2)	0.0014 (15)	0.0147 (16)	0.0015 (16)
04	0.029 (2)	0.0196 (18)	0.037 (2)	0.0035 (15)	0.0198 (19)	0.0025 (16)
05	0.0261 (19)	0.0220 (18)	0.0282 (19)	-0.0037 (15)	0.0150 (16)	0.0015 (15)
06	0.030 (2)	0.0274 (19)	0.0267 (19)	0.0042 (16)	0.0204 (17)	0.0027 (16)
07	0.0254 (18)	0.0252 (19)	0.0233 (18)	0.0035 (15)	0.0147 (16)	0.0041 (15)
08	0.0235 (18)	0.0240 (18)	0.0255 (19)	-0.0027 (15)	0.0136 (16)	-0.0021 (15)
09	0.0157 (16)	0.0276 (19)	0.0241 (18)	-0.0007 (15)	0.0058 (14)	-0.0019 (16)
O10	0.0233 (18)	0.0223 (18)	0.0277 (19)	0.0027 (14)	0.0141 (16)	-0.0004 (15)
011	0.0218 (17)	0.0216 (17)	0.0166 (15)	0.0026 (14)	0.0102 (14)	0.0004 (13)
012	0.0182 (16)	0.0186 (16)	0.0233 (17)	0.0029 (13)	0.0099 (14)	0.0012 (14)
013	0.0200 (16)	0.0220 (17)	0.0162 (15)	0.0041 (14)	0.0093 (14)	0.0017 (13)
014	0.0184 (17)	0.0242 (18)	0.0216 (17)	-0.0004(14)	0.0100 (15)	0.0019 (14)
015	0.0243 (19)	0.0237 (19)	0.0263 (19)	-0.0024(15)	0.0132 (16)	-0.0021(15)
016	0.031 (2)	0.0213 (18)	0.027 (2)	0.0015 (16)	0.0171 (17)	-0.0018(15)
017	0.0229 (18)	0.0236 (19)	0.0225 (18)	-0.0043(15)	0.0094 (15)	-0.0048(15)
018	0.0260 (19)	0.0245 (19)	0.027 (2)	-0.0025(15)	0.0145 (17)	-0.0060(16)
N1	0.039 (3)	0.058 (4)	0.052 (4)	-0.007(3)	0.033 (3)	-0.003(3)
N2	0.045 (3)	0.047 (4)	0.056 (4)	0.017 (3)	0.033 (3)	0.026 (3)
C1	0.027 (3)	0.038 (3)	0.028 (3)	0.005 (2)	0.017 (2)	0.003 (2)
C2	0.028 (3)	0.047 (4)	0.039 (4)	-0.002(3)	0.016 (3)	0.000 (3)
C3	0.060 (5)	0.034 (4)	0.058 (5)	-0.010 (3)	0.038 (4)	0.002 (3)
C4	0.040 (3)	0.022 (3)	0.038 (3)	0.007 (2)	0.017 (3)	0.011 (2)
C5	0.037 (4)	0.066 (5)	0.029 (3)	0.021 (3)	0.016 (3)	-0.001(3)
N3	0.067 (4)	0.032 (3)	0.057 (4)	0.005 (3)	0.041 (4)	0.008 (3)
N4	0.055 (4)	0.025 (3)	0.037 (3)	-0.011 (2)	0.028 (3)	0.000 (2)
C6	0.032 (3)	0.024 (3)	0.034 (3)	0.001 (2)	0.019 (3)	0.001 (2)
C7	0.033 (3)	0.034 (3)	0.031 (3)	0.000 (2)	0.017 (3)	0.006 (2)
C8	0.033 (3)	0.027 (3)	0.052 (4)	-0.001 (3)	0.020 (3)	0.006 (3)
C9	0.030 (3)	0.023 (3)	0.028 (3)	-0.002 (2)	0.013 (2)	-0.007 (2)
C10	0.061 (5)	0.037 (4)	0.038 (4)	0.001 (3)	0.027 (4)	-0.009(3)
N5	0.059 (4)	0.046 (4)	0.051 (4)	0.000 (3)	0.027 (4)	-0.005(3)
N6	0.089 (5)	0.022 (3)	0.039 (3)	-0.005 (3)	0.021 (4)	0.006 (2)
C11	0.040 (3)	0.022 (3)	0.032 (3)	0.001 (2)	0.012 (3)	0.000 (2)
C12	0.062 (5)	0.028 (3)	0.035 (4)	0.008 (3)	0.013 (3)	-0.001 (3)
C13	0.058 (5)	0.024 (3)	0.052 (5)	0.003 (3)	0.010 (4)	0.001 (3)
C14	0.042 (4)	0.023 (3)	0.033 (3)	0.001 (3)	0.010 (3)	0.013 (2)
C15	0.049 (4)	0.046 (4)	0.035 (4)	0.004 (3)	0.013 (3)	0.012 (3)
N7	0.047 (4)	0.054 (4)	0.042 (3)	-0.007 (3)	0.023 (3)	0.000 (3)
N8	0.066 (4)	0.031 (3)	0.031 (3)	-0.014 (3)	0.015 (3)	-0.002(2)
C16	0.034 (3)	0.029 (3)	0.032 (3)	0.000 (3)	0.013 (3)	0.001 (2)
C17	0.066 (5)	0.028 (3)	0.030 (3)	0.000 (3)	0.023 (3)	0.009 (3)
C18	0.057 (5)	0.040 (4)	0.028 (3)	0.006 (3)	0.011 (3)	-0.003 (3)
C19	0.031 (3)	0.025 (3)	0.034 (3)	-0.001 (2)	0.008 (3)	-0.011 (2)
C20	0.037 (4)	0.023 (3)	0.058 (5)	-0.006 (3)	0.021 (3)	-0.004 (3)
N9	0.050 (4)	0.053 (4)	0.092 (6)	-0.011 (3)	0.051 (4)	-0.005 (4)

N10	0.061 (4)	0.036 (3)	0.067 (5)	0.008 (3)	0.038 (4)	0.018 (3)
C21	0.030 (3)	0.033 (3)	0.031 (3)	-0.001 (2)	0.018 (2)	0.007 (2)
C22	0.030 (3)	0.044 (4)	0.056 (4)	-0.005 (3)	0.031 (3)	-0.004 (3)
C23	0.056 (4)	0.040 (4)	0.040 (4)	-0.021 (3)	0.031 (4)	-0.004 (3)
C24	0.036 (3)	0.016 (2)	0.033 (3)	0.004 (2)	0.012 (3)	0.005 (2)
C25	0.027 (3)	0.046 (4)	0.053 (4)	0.011 (3)	0.014 (3)	-0.001 (3)

Geometric parameters (Å, °)

V1-01E	1.595 (4)	Te1—O15	1.769 (4)
V101	1.814 (4)	Te1—O18	1.774 (4)
V1—O2	1.867 (4)	Te1—O14	1.931 (4)
V1-05	1.884 (4)	Te1—O13	1.950 (4)
V1-015	2.067 (4)	Te1—O2C	2.052 (4)
V1-01C	2.374 (4)	Te1—O1C	2.063 (4)
V2—O2E	1.601 (4)	Te2—O17	1.774 (4)
V2—O4	1.816 (4)	Te2—O16	1.789 (4)
V2—O2	1.818 (4)	Te2—O11	1.916 (4)
V2—O12	2.022 (4)	Te2—O12	1.923 (4)
V2—014	2.039 (4)	Te2—O1C	2.048 (4)
V201C	2.287 (4)	Te2—O2C	2.052 (4)
V3—O3E	1.611 (4)	N1—C5	1.347 (10)
V3—01	1.824 (4)	N1—C1	1.409 (8)
V3—O4	1.848 (4)	N2—C1	1.307 (8)
V3—O6	1.901 (4)	C1—C2	1.420 (9)
V3—016	2.041 (4)	C2—C3	1.343 (10)
V3—01C	2.429 (4)	C3—C4	1.321 (10)
V4—O6	1.809 (4)	C4—C5	1.325 (11)
V4—05	1.816 (4)	N3—C10	1.366 (10)
V4—011	2.030 (4)	N3—C6	1.411 (9)
V4—O13	2.080 (4)	N4—C6	1.330 (8)
V401C	2.285 (4)	C6—C7	1.410 (8)
V5—O5E	1.601 (4)	C7—C8	1.345 (10)
V5—07	1.808 (4)	C8—C9	1.324 (9)
V5—08	1.810 (4)	C9—C10	1.334 (10)
V5—O14	2.034 (4)	N5—C15	1.330 (10)
V5—012	2.045 (4)	N5—C11	1.425 (9)
V5—O2C	2.277 (4)	N6—C11	1.322 (8)
V6—06E	1.596 (4)	C11—C12	1.381 (9)
V6—09	1.813 (4)	C12—C13	1.361 (10)
V6—O10	1.815 (4)	C13—C14	1.323 (11)
V6—O13	2.022 (4)	C14—C15	1.341 (10)
V6—011	2.046 (4)	N7—C20	1.357 (9)
V6—O2C	2.296 (4)	N7—C16	1.444 (9)
V7—07E	1.610 (4)	N8—C16	1.319 (8)
V7—O3	1.810 (4)	C16—C17	1.408 (9)
V7—O10	1.871 (4)	C17—C18	1.364 (10)
V7—07	1.879 (4)	C18—C19	1.331 (10)

V7—O18	2.058 (4)	C19—C20	1.322 (10)
V7—02C	2.396 (4)	N9—C25	1.379 (10)
V8-08E	1 603 (4)	N9—C21	1 404 (9)
V8-03	1 835 (4)	N10-C21	1 320 (8)
V8-09	1.833(4)	C_{21}	1.320(0) 1.430(9)
V8 08	1.045(4) 1.018(4)	C^{22} C^{23}	1.450(9)
V8_017	2.031(4)	$C_{22} = C_{23}$	1.331(10) 1.316(10)
V8_02C	2.031(4)	$C_{23} = C_{24}$	1.310(10) 1.300(10)
V 8-02C	2.414 (4)	024-023	1.309 (10)
01F—V1—01	104.6(2)	015—Te1—013	95 61 (17)
OIE VI OI	104.0(2) 104.1(2)	018 Te1 013	95.62 (17)
01 - V1 - 02	91.42(19)	014—Te1—013	158 89 (16)
O1E V1 $O5$	101.7(2)	015 Te1 02C	166 18 (16)
01 - V1 = 05	101.7(2) 00.34(10)	013 - 1e1 - 02C	88.46 (16)
01 - 1 - 05	50.34(19)	018 - 1e1 - 02C	88.40 (10)
$02 - \sqrt{1 - 05}$	132.70(17)	014 - 101 - 020	81.97(13)
OIE VI OIS	99.0 (2) 155.70 (19)	013 - 101 - 020	81.48 (13)
01 - v1 - 015	155.70(18)		88.51 (16)
02-V1-015	84.15 (18)		166.14 (16)
05-1-015	83.16 (17)		82.10 (15)
OIE—VI—OIC	173.4 (2)	013—1e1—01C	81.65 (15)
01—V1—01C	81.78 (16)	O2C—Te1—O1C	77.71 (14)
02—V1—01C	76.99 (15)	O17—Te2—O16	104.49 (18)
05—V1—01C	76.40 (15)	O17—Te2—O11	96.53 (17)
015—V1—01C	73.94 (14)	O16—Te2—O11	97.11 (17)
O2E—V2—O4	105.1 (2)	O17—Te2—O12	96.35 (17)
O2E—V2—O2	105.0 (2)	O16—Te2—O12	95.45 (17)
O4—V2—O2	93.47 (19)	O11—Te2—O12	159.15 (16)
O2E-V2-O12	99.83 (19)	O17—Te2—O1C	166.67 (16)
O4—V2—O12	90.20 (17)	O16—Te2—O1C	88.83 (17)
O2—V2—O12	152.94 (17)	O11—Te2—O1C	81.94 (15)
O2E-V2-O14	99.1 (2)	O12—Te2—O1C	81.75 (15)
O4—V2—O14	153.70 (17)	O17—Te2—O2C	88.63 (16)
O2—V2—O14	90.08 (17)	O16—Te2—O2C	166.84 (17)
O12—V2—O14	75.45 (15)	O11—Te2—O2C	82.04 (14)
O2E—V2—O1C	171.85 (19)	O12—Te2—O2C	81.94 (15)
04—V2—01C	80.48 (16)	O1C—Te2— $O2C$	78.04 (14)
02 - V2 - 01C	80.23 (16)	$Te^2 - O1C - Te^1$	102.01 (15)
012 - V2 - 01C	73 96 (14)	$Te^2 = 01C = V4$	94 00 (14)
012 V2 010	74 46 (14)	Te1 $-01C$ V4	95.66 (14)
$0.3F - V_{3} - 0.1$	105.6(2)	$T_{e2} = 01C = V2$	94 16 (14)
$O_{3E} = V_{3} = O_{1}$	103.0(2) 104.6(2)	$T_{e1} = 01C = V2$	94.10(14)
$03E = \sqrt{3} = 04$	104.0(2)	$V_{4} = 01C = V_{2}$	165 78 (17)
$01 - \sqrt{3} - 04$	102.5(2)	$V_{1} = 01C = V_{2}$	105.76(17)
01 V3 06	103.3(2) 80 30 (10)	$\frac{102-01C-V1}{102}$	80 03 (12)
$01 - \sqrt{3} - 00$	(17)	$V_{4} = 01C = V_{1}$	95.03(13)
04 - 100	100.0(1)	$V_{1} = V_{1}$	03.12(12)
$03E = \sqrt{3} = 010$	100.9(2)	$v_2 = 01C = v_1$ T ₂ 2 01C V2	04.04 (12)
$01 - \sqrt{3} - 010$	133.48 (17)	162 - 010 - V3	08.27 (13)
U4—V3—U16	84.20(1/)	1e1 - 01C - V3	169.63 (18)

O6—V3—O16	82.68 (17)	V4—O1C—V3	84.84 (12)
O3E—V3—O1C	174.3 (2)	V2—O1C—V3	83.79 (12)
01—V3—01C	80.04 (15)	V1-01C-V3	80.69 (11)
04—V3—01C	76.06 (15)	Te2—O2C—Te1	102.24 (15)
$06 - V_3 - 01C$	75 12 (15)	$Te^2 - O^2C - V_5$	94 46 (14)
$016 - V_3 - 01C$	73 48 (14)	Te1 $-02C-V5$	94 28 (14)
$0.4F - V_4 - 0.6$	105.1 (2)	$Te^2 - \Omega^2 C - V6$	94 38 (14)
O4E - V4 = O5	103.1(2) 104.1(2)	$Te1_02C_V6$	94 46 (13)
04L V4 05	95 27 (19)	$V_{2} = 0.02 = 0.000$	165 98 (17)
O4E V4 O11	100.81(10)	$T_{\rm P}^2 = 0.2C = V_0^2$	163.78(17)
04E = 04 = 011	100.01(19) 80.02(17)	$T_{c2} = 0.2 C = \sqrt{7}$	100.70(10)
05 V4 011	39.92(17) 152 10(17)	$V_{2} = 0.02$ V7	88.98(13)
$03 - \sqrt{4} - 011$	132.19(17)	$\sqrt{3}$	84.49(12)
04E - V4 - 013	99.75(19)	$V_0 = 0.2 C = V/$	84.75 (12)
06	132.95(17)	$1e_2 - 0_2 C - v_8$	88.04 (13)
$05 - \sqrt{4} - 013$	88.79 (16)	1e1 - 02C - V8	169.69 (18)
011	/4.93 (15)	V5—02C—V8	85.54 (12)
O4E—V4—OIC	172.39 (18)	V6—02C—V8	83.91 (12)
06—V4—01C	80.60 (16)	V7—O2C—V8	80.74 (11)
05—V4—01C	80.03 (15)	V1—O1—V3	117.4 (2)
011—V4—01C	73.89 (14)	V2—O2—V1	116.8 (2)
O13—V4—O1C	73.76 (14)	V7—O3—V8	117.5 (2)
O5E—V5—O7	104.3 (2)	V2—O4—V3	118.6 (2)
O5E—V5—O8	104.1 (2)	V4—O5—V1	116.8 (2)
O7—V5—O8	95.22 (18)	V4—O6—V3	118.0 (2)
O5E—V5—O14	99.98 (19)	V5—O7—V7	116.9 (2)
O7—V5—O14	89.63 (17)	V5—O8—V8	117.5 (2)
O8—V5—O14	153.42 (17)	V6—O9—V8	119.0 (2)
O5E-V5-012	100.09 (19)	V6—O10—V7	118.1 (2)
O7—V5—O12	153.11 (17)	Te2-O11-V4	107.03 (17)
O8—V5—O12	89.60 (16)	Te2-O11-V6	107.39 (17)
O14—V5—O12	75.06 (15)	V4—O11—V6	101.05 (16)
O5E—V5—O2C	172.62 (18)	Te2—O12—V2	107.36 (17)
O7—V5—O2C	80.70 (15)	Te2-012-V5	106.61 (17)
O8—V5—O2C	80.62 (16)	V2—012—V5	101.10 (17)
O14—V5—O2C	74.39 (14)	Te1-013-V6	107.13 (18)
O12—V5—O2C	74.01 (14)	Te1-013-V4	106.28 (16)
O6E—V6—O9	105.6 (2)	V6—O13—V4	100.15 (15)
O6E—V6—O10	104.8 (2)	Te1-014-V5	106.48 (17)
09—V6—010	93.46 (18)	Te1-014-V2	106.64 (17)
06E—V6—013	99.6 (2)	V5-014-V2	100.86(17)
09 - V6 - 013	$152\ 42\ (17)$	$Te1_015_V1$	108.51(19)
010 - V6 - 013	90.62 (16)	$Te^2 - 016 - V3$	100.51(1)
06F - V6 - 011	1010(2)	$Te^2 = 0.17 = V8$	109.7(2)
09—V6—011	88 47 (17)	Te1-018-V7	109 11 (19)
010 - V6 - 011	152 55 (17)	C_{5} N1—C1	1197(6)
013 - V6 - 011	75 85 (15)	N_2 —C1—N1	122 8 (6)
O6E V6 O1	172 43 (10)	$N_2 - C_1 - C_2$	121.3 (6)
09 - V6 - 02C	79 70 (16)	N1_C1_C2	121.3(0) 115 9(6)
0 = 10 - 020	12.10 (10)	111 - 01 - 02	112.2(0)

010—V6—02C	79 87 (16)	$C_{3} - C_{2} - C_{1}$	120 3 (7)
013 - V6 - 02C	74.19 (14)	C4—C3—C2	120.3(7) 121.4(7)
011—V6—02C	73.54 (14)	C3—C4—C5	120.7 (6)
07E—V7—03	104.7 (2)	C4—C5—N1	122.1(7)
O7E—V7—O10	104.1 (2)	C10—N3—C6	120.7 (6)
O3—V7—O10	90.59 (18)	N4—C6—C7	121.6 (6)
O7E—V7—O7	102.8 (2)	N4—C6—N3	122.3 (6)
O3—V7—O7	90.85 (18)	C7—C6—N3	116.1 (6)
O10—V7—O7	151.82 (17)	C8—C7—C6	119.6 (6)
O7E—V7—O18	100.5 (2)	C9—C8—C7	122.6 (6)
O3—V7—O18	154.80 (17)	C8—C9—C10	120.7 (6)
O10—V7—O18	83.70 (17)	C9—C10—N3	120.2 (7)
O7—V7—O18	83.10 (17)	C15—N5—C11	120.3 (7)
O7E—V7—O2C	173.89 (19)	N6-C11-C12	122.2 (6)
O3—V7—O2C	81.35 (15)	N6—C11—N5	121.1 (6)
O10—V7—O2C	76.18 (15)	C12—C11—N5	116.6 (6)
O7—V7—O2C	76.23 (15)	C13—C12—C11	120.0 (7)
O18—V7—O2C	73.45 (14)	C14—C13—C12	121.4 (7)
O8E—V8—O3	105.8 (2)	C13—C14—C15	120.6 (6)
O8E—V8—O9	103.5 (2)	N5-C15-C14	121.1 (7)
O3—V8—O9	91.99 (18)	C20—N7—C16	119.0 (6)
O8E—V8—O8	104.8 (2)	N8—C16—C17	122.6 (6)
O3—V8—O8	88.41 (18)	N8—C16—N7	120.6 (6)
O9—V8—O8	150.53 (17)	C17—C16—N7	116.8 (6)
O8E—V8—O17	100.3 (2)	C18—C17—C16	119.2 (6)
O3—V8—O17	153.80 (17)	C19—C18—C17	122.1 (7)
O9—V8—O17	84.52 (17)	C20—C19—C18	121.1 (6)
O8—V8—O17	82.30 (16)	C19—C20—N7	121.9 (7)
O8E—V8—O2C	173.9 (2)	C25—N9—C21	119.3 (6)
O3—V8—O2C	80.36 (15)	N10—C21—N9	122.3 (6)
O9—V8—O2C	75.98 (14)	N10-C21-C22	121.9 (6)
O8—V8—O2C	75.05 (14)	N9—C21—C22	115.8 (6)
O17—V8—O2C	73.59 (14)	C23—C22—C21	119.5 (6)
O15—Te1—O18	105.31 (18)	C24—C23—C22	122.7 (6)
O15—Te1—O14	97.35 (17)	C25—C24—C23	120.0 (6)
O18—Te1—O14	96.93 (18)	C24—C25—N9	122.5 (6)

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H···A
N1—H1…O6 ⁱ	0.86	2.57	3.426 (8)	172
N2—H2A····O1 ⁱ	0.86	2.26	3.105 (8)	167
N2—H2 <i>B</i> ···O3 ⁱⁱ	0.86	2.50	3.006 (7)	118
N2—H2 <i>B</i> ···O10 ⁱⁱ	0.86	2.28	3.121 (8)	165
C4—H4…O3 <i>E</i>	0.93	2.44	2.995 (8)	119
C4—H4…O8 <i>E</i> ⁱⁱⁱ	0.93	2.26	3.073 (8)	146
С5—Н5…О9ііі	0.93	2.24	3.136 (8)	161
N3—H3A····O12 ^{iv}	0.86	2.54	3.397 (7)	175

N4—H4A····O7 ^v	0.86	2.05	2.896 (7)	168
N4—H4 <i>B</i> ···O16 ^{iv}	0.86	2.19	2.998 (7)	156
C7—H7…O18 ^v	0.93	2.57	3.495 (8)	171
C9—H9…O5 ⁱ	0.93	1.86	2.760 (7)	161
N5—H5 <i>A</i> ···O10 ⁱⁱ	0.86	2.61	3.404 (8)	154
N6—H6 A ···O1 E^{vi}	0.86	2.14	2.922 (8)	151
N6—H6 B ···O7 E^{ii}	0.86	2.05	2.900 (8)	171
C12—H12…O1 <i>E</i> ^{vi}	0.93	2.63	3.312 (9)	130
C14—H14…O8 ^{iv}	0.93	1.78	2.703 (7)	174
C14—H14…O17 ^{iv}	0.93	2.62	3.146 (8)	117
N7—H7A····O15 ^{vi}	0.86	2.48	3.308 (8)	161
N8—H8A····O3E ^{vii}	0.86	2.12	2.966 (7)	169
N8—H8 <i>B</i> …O14 ^{vi}	0.86	2.18	2.963 (7)	152
C19—H19…O13 ⁱⁱ	0.93	1.88	2.788 (7)	165
C20—H20…O18 ⁱⁱ	0.93	2.43	3.202 (8)	140
N9—H9 <i>A</i> ···O5 <i>E</i>	0.86	2.46	3.244 (7)	151
N10—H10A…O3	0.86	2.30	3.098 (8)	155
N10—H10 <i>B</i> ···O1 ^{viii}	0.86	2.65	3.294 (8)	132
N10—H10 <i>B</i> ····O2 ^{viii}	0.86	2.34	3.169 (8)	162
C22—H22···O2 E^{viii}	0.93	2.29	3.189 (8)	164
C24—H24····O4 E^{ix}	0.93	2.35	2.929 (7)	120
C24—H24····O6 <i>E</i> ^{ix}	0.93	2.61	3.153 (7)	118
C24—H24…O11 ^x	0.93	2.48	3.003 (7)	116
C10—H10…Cg1	0.93	3.07	3.902	151
C18—H18…Cg5 ^{iv}	0.93	2.66	3.450	143

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