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# Crystal structure of di-$\mu$-methanolato-bis{[$N'$-(1-benzoylprop-1-en-2-yl)thiophene-2-carbohydrazidato-$\kappa^3O,N',O'$]-oxidovanadium(V)}

**Murilo C. Carroccia,[a] Rafaela B. P. Pesci,[a] Pedro Ivo da S. Maia[b] and Victor M. Deflon[a]***

[a]Instituto de Química de São Carlos, Universidade de São Paulo, 13560-970, São Carlos, SP, Brazil, and [b]Departamento de Química, Universidade Federal do Triângulo Mineiro, 38025-440, Uberaba, MG, Brazil. *Correspondence e-mail: deflon@iqsc.usp.br

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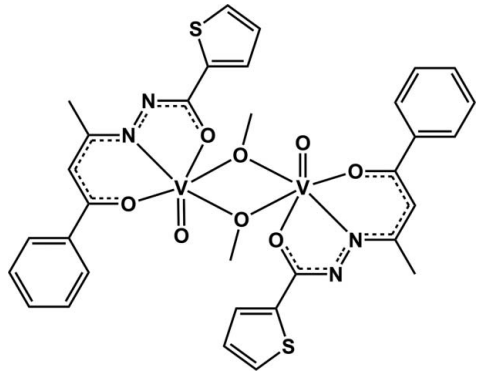
The neutral binuclear molecule of the title complex, $[V_2(C_{15}H_{12}N_2O_2S)_2(CH_3O)_2O_2]$, exhibits inversion symmetry and consists of two oxidovanadium(V) $(VO)^{3+}$ fragments, each coordinated by a dianionic and $O,N',O'$-chelating $N'$-(1-benzoylprop-1-en-2-yl)thiophene-2-carbohydrazidate ligand. The $V^{5+}$ cations are bridged by two asymmetrically bonding methanolate ligands [V—O = 1.8155 (12) and 2.3950 (13) Å] originating from the deprotonation of the methanol solvent. The coordination sphere of the $V^V$ atom is distorted octahedral, with the equatorial plane defined by the three donor atoms of the thiophene-2-carbohydrazidate ligand and the O atom of a methanolate unit. The axial positions are occupied by the oxide group and the remaining methanolate ligand. The axially bound methanolate ligand shows a longer V—O bond length due to the *trans* influence caused by the tightly bonded oxide group. The packing of the complex molecules is dominated by dispersion forces.

**Keywords:** crystal structure; thiophene-2-carbohydrazide; vanadium(V) complex; dinuclear complex; alkoxide bridging.

**CCDC reference**: 1023545

## 1. Related literature

For related structures of binuclear vanadium(V) complexes with $O,N,O$-chelating hydrazonate ligands and methanolate bridges, see: Sarkar & Pal (2009); Monfared *et al.* (2011); Maia *et al.* (2005, 2007). For synthetic details, see: Mondal *et al.* (2008).



## 2. Experimental

### 2.1. Crystal data

$[V_2(C_{15}H_{12}N_2O_2S)_2(CH_3O)_2O_2]$
$M_r$ = 764.60
Monoclinic, $P2_1/n$
$a$ = 10.9900 (2) Å
$b$ = 15.9297 (3) Å
$c$ = 11.0178 (3) Å
$\beta$ = 119.884 (1)°
$V$ = 1672.39 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.74 mm$^{-1}$
$T$ = 296 K
0.21 × 0.21 × 0.10 mm

### 2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.860, $T_{max}$ = 0.930
20108 measured reflections
3067 independent reflections
2718 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.083
$S$ = 1.04
3067 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

## Acknowledgements

The authors thank FAPESP (grant Nos. 2009/54011-8, 2011/16160-1 and 2011/16380-1), FAPEMIG, CNPq and CAPES for supporting this work.

Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5059).

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# supporting information

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# Crystal structure of di-$\mu$-methanolato-bis{[*N*′-(1-benzoylprop-1-en-2-yl)thiophene-2-carbohydrazidato-$\kappa^3O,N',O'$]oxidovanadium(V)}

**Murilo C. Carroccia, Rafaela B. P. Pesci, Pedro Ivo da S. Maia and Victor M. Deflon**

## S1. Experimental

The synthesis of the complex was developed by a slight modification of the procedure previously described by Mondal *et al.* (2008). 0.2 mmol (0.053 g) of [VO(acac)$_2$] and 0.2 mmol of benzoylacetone-2-thinoylhydrazone (0.058 g) were diluted separately in methanol. The solutions were mixed and stirred for 0.5 h. A brown solution was obtained and after slow evaporation of the solvent single crystals were formed.

## S2. Refinement

The H atoms were positioned geometrically and refined using a riding model with C—H bond lengths of 0.96 Å (methyl) and of 0.93 Å (aromatic) and with $U_{iso}$(H) = 1.5$U_{eq}$(C) (methyl), and with $U_{iso}$(H) = 1.2$U_{eq}$(C) (aromatic).

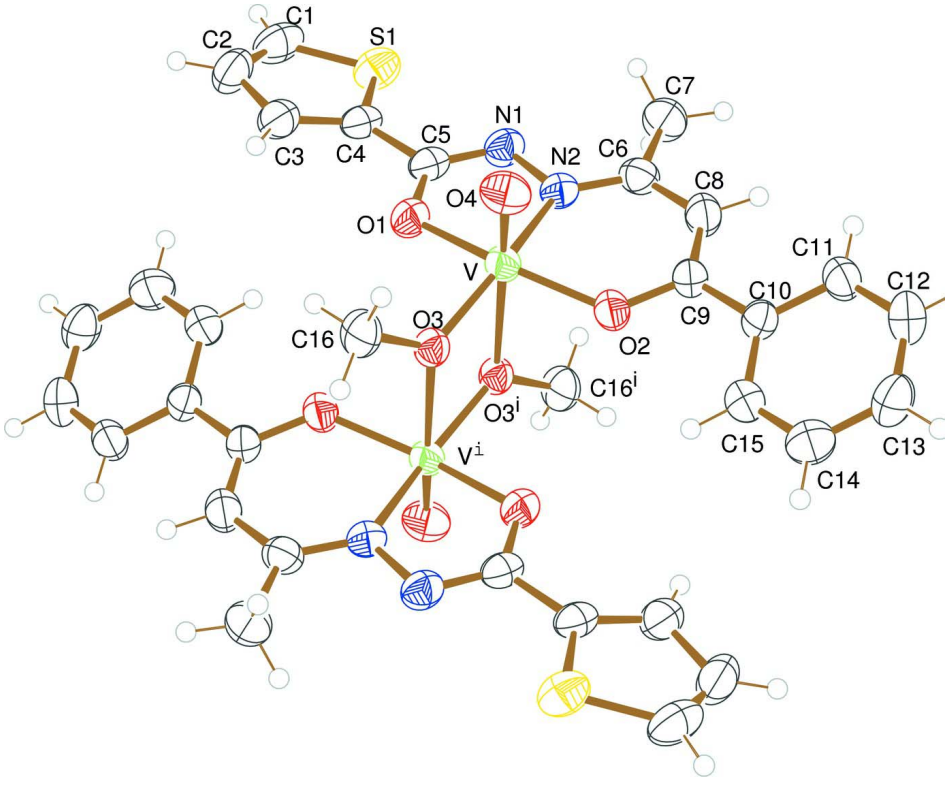


**Figure 1**

The binuclear molecular structure of the title compound with atom labels and displacement ellipsoids drawn at the 50% probability level. [Symmettry code: i) -*x*, -*y*+2, -*z*+1.]

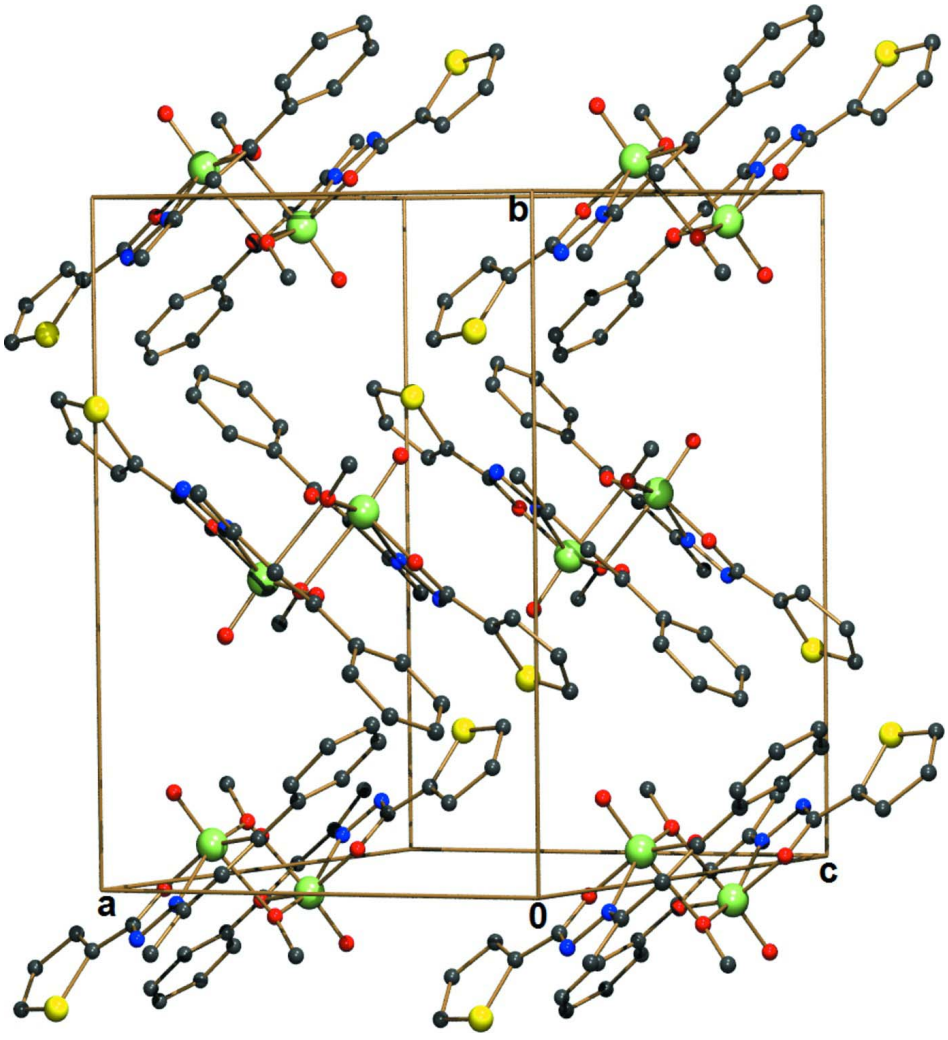


**Figure 2**

Packing diagram of the title complex. No hydrogen-bonding interactions are observed.

**Di-$\mu$-methanolato-$\kappa^4O$:$O$-bis{[$N'$-(1-benzoylprop-1-en-2-yl)thiophene-2-carbohydrazidato-$\kappa^3O,N',O'$]oxidovanadium(V)}**

*Crystal data*

$[V_2(C_{15}H_{12}N_2O_2S)_2(CH_3O)_2O_2]$
$M_r$ = 764.60
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 10.9900 (2) Å
$b$ = 15.9297 (3) Å
$c$ = 11.0178 (3) Å
$\beta$ = 119.884 (1)°
$V$ = 1672.39 (6) Å$^3$
$Z$ = 2
$F(000)$ = 784
$D_x$ = 1.518 Mg m$^{-3}$
Melting point: 451 K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9900 reflections
$\theta$ = 2.5–25.4°
$\mu$ = 0.74 mm$^{-1}$
$T$ = 296 K
Prism, brown
0.21 × 0.21 × 0.10 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.860, $T_{max}$ = 0.930
20108 measured reflections
3067 independent reflections
2718 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020
$\theta_{max}$ = 25.4°, $\theta_{min}$ = 2.1°
$h$ = −13→13
$k$ = −19→19
$l$ = −10→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.083
$S$ = 1.04
3067 reflections
219 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
$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.7671P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

*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 $F^2 > \sigma(F^2)$ 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| V | −0.01766 (3) | 0.95609 (2) | 0.63227 (3) | 0.03545 (12) |
| S1 | −0.33170 (6) | 1.19868 (4) | 0.71561 (6) | 0.05580 (17) |
| O2 | 0.17270 (14) | 0.93610 (9) | 0.73088 (13) | 0.0449 (3) |
| O3 | −0.06694 (12) | 0.93265 (8) | 0.45226 (12) | 0.0362 (3) |
| O4 | −0.07281 (16) | 0.87680 (9) | 0.67733 (15) | 0.0525 (4) |
| N2 | 0.02549 (16) | 1.03306 (10) | 0.80379 (16) | 0.0382 (4) |
| N1 | −0.08298 (17) | 1.08675 (10) | 0.78577 (17) | 0.0426 (4) |
| C9 | 0.26550 (19) | 0.93078 (12) | 0.86578 (19) | 0.0387 (4) |
| C8 | 0.2507 (2) | 0.97723 (14) | 0.9611 (2) | 0.0463 (5) |
| H7 | 0.3208 | 0.9727 | 1.0544 | 0.056* |
| C6 | 0.1366 (2) | 1.03221 (13) | 0.9298 (2) | 0.0417 (4) |
| C7 | 0.1447 (2) | 1.08777 (15) | 1.0428 (2) | 0.0539 (5) |
| H2 | 0.2270 | 1.0740 | 1.1299 | 0.081* |
| H3 | 0.0628 | 1.0797 | 1.0515 | 0.081* |
| H1 | 0.1496 | 1.1453 | 1.0198 | 0.081* |
| C5 | −0.1873 (2) | 1.07576 (12) | 0.6604 (2) | 0.0389 (4) |

| | | | | |
|---|---|---|---|---|
| O1 | −0.18078 (14) | 1.02693 (9) | 0.56828 (14) | 0.0436 (3) |
| C4 | −0.3193 (2) | 1.11904 (12) | 0.6175 (2) | 0.0404 (4) |
| C1 | −0.5054 (3) | 1.21073 (16) | 0.6013 (3) | 0.0607 (6) |
| H6 | −0.5611 | 1.2508 | 0.6118 | 0.073* |
| C2 | −0.5541 (2) | 1.15642 (17) | 0.4942 (3) | 0.0603 (6) |
| H4 | −0.6476 | 1.1540 | 0.4238 | 0.072* |
| C3 | −0.4478 (2) | 1.10288 (14) | 0.4995 (2) | 0.0473 (5) |
| H5 | −0.4625 | 1.0625 | 0.4326 | 0.057* |
| C10 | 0.38325 (19) | 0.87296 (12) | 0.89970 (19) | 0.0380 (4) |
| C15 | 0.4093 (2) | 0.84603 (14) | 0.7951 (2) | 0.0473 (5) |
| H12 | 0.3543 | 0.8661 | 0.7043 | 0.057* |
| C14 | 0.5155 (2) | 0.79008 (16) | 0.8240 (2) | 0.0586 (6) |
| H11 | 0.5325 | 0.7730 | 0.7532 | 0.070* |
| C13 | 0.5968 (2) | 0.75917 (15) | 0.9579 (2) | 0.0552 (6) |
| H10 | 0.6685 | 0.7212 | 0.9773 | 0.066* |
| C12 | 0.5717 (2) | 0.78462 (14) | 1.0622 (2) | 0.0506 (5) |
| H9 | 0.6258 | 0.7630 | 1.1520 | 0.061* |
| C11 | 0.4678 (2) | 0.84163 (13) | 1.03576 (19) | 0.0453 (5) |
| H8 | 0.4534 | 0.8595 | 1.1079 | 0.054* |
| C16 | −0.1838 (2) | 0.88198 (14) | 0.3600 (2) | 0.0493 (5) |
| H15 | −0.1841 | 0.8314 | 0.4072 | 0.074* |
| H13 | −0.1768 | 0.8680 | 0.2789 | 0.074* |
| H14 | −0.2692 | 0.9124 | 0.3317 | 0.074* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| V | 0.03501 (19) | 0.0397 (2) | 0.03146 (18) | 0.00311 (13) | 0.01640 (14) | −0.00117 (12) |
| S1 | 0.0529 (3) | 0.0550 (3) | 0.0687 (4) | 0.0045 (3) | 0.0372 (3) | −0.0054 (3) |
| O2 | 0.0387 (7) | 0.0601 (9) | 0.0324 (7) | 0.0123 (6) | 0.0151 (6) | 0.0024 (6) |
| O3 | 0.0319 (7) | 0.0404 (7) | 0.0327 (6) | −0.0024 (5) | 0.0133 (5) | −0.0056 (5) |
| O4 | 0.0642 (10) | 0.0465 (8) | 0.0544 (8) | −0.0015 (7) | 0.0355 (8) | 0.0020 (7) |
| N2 | 0.0374 (9) | 0.0420 (9) | 0.0391 (8) | 0.0022 (7) | 0.0220 (7) | −0.0014 (7) |
| N1 | 0.0407 (9) | 0.0434 (9) | 0.0484 (9) | 0.0061 (7) | 0.0258 (8) | −0.0007 (7) |
| C9 | 0.0328 (10) | 0.0459 (11) | 0.0339 (9) | 0.0006 (8) | 0.0141 (8) | 0.0041 (8) |
| C8 | 0.0390 (11) | 0.0566 (12) | 0.0359 (10) | 0.0057 (9) | 0.0131 (8) | −0.0022 (9) |
| C6 | 0.0444 (11) | 0.0468 (11) | 0.0368 (10) | −0.0043 (9) | 0.0224 (9) | −0.0040 (8) |
| C7 | 0.0558 (13) | 0.0607 (14) | 0.0454 (11) | −0.0017 (11) | 0.0256 (10) | −0.0133 (10) |
| C5 | 0.0395 (10) | 0.0371 (10) | 0.0486 (11) | 0.0018 (8) | 0.0285 (9) | 0.0045 (8) |
| O1 | 0.0362 (7) | 0.0522 (8) | 0.0435 (7) | 0.0058 (6) | 0.0207 (6) | −0.0018 (6) |
| C4 | 0.0411 (11) | 0.0397 (10) | 0.0504 (11) | 0.0018 (8) | 0.0304 (9) | 0.0054 (8) |
| C1 | 0.0559 (14) | 0.0571 (14) | 0.0868 (17) | 0.0149 (11) | 0.0489 (14) | 0.0092 (13) |
| C2 | 0.0365 (11) | 0.0722 (16) | 0.0692 (15) | 0.0081 (11) | 0.0242 (11) | 0.0161 (13) |
| C3 | 0.0426 (11) | 0.0502 (12) | 0.0530 (11) | 0.0017 (9) | 0.0268 (10) | 0.0031 (10) |
| C10 | 0.0314 (9) | 0.0420 (10) | 0.0370 (9) | −0.0013 (8) | 0.0144 (8) | 0.0006 (8) |
| C15 | 0.0434 (11) | 0.0582 (13) | 0.0381 (10) | 0.0049 (10) | 0.0186 (9) | 0.0035 (9) |
| C14 | 0.0568 (14) | 0.0690 (15) | 0.0573 (13) | 0.0109 (12) | 0.0341 (11) | −0.0018 (11) |
| C13 | 0.0409 (12) | 0.0560 (13) | 0.0616 (13) | 0.0113 (10) | 0.0202 (10) | 0.0004 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C12 | 0.0414 (11) | 0.0503 (12) | 0.0429 (11) | 0.0047 (9) | 0.0079 (9) | 0.0019 (9) |
| C11 | 0.0433 (11) | 0.0535 (12) | 0.0335 (9) | 0.0052 (9) | 0.0150 (8) | 0.0005 (8) |
| C16 | 0.0420 (11) | 0.0522 (12) | 0.0445 (11) | −0.0140 (9) | 0.0145 (9) | −0.0093 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| V—O4 | 1.5839 (15) | C5—O1 | 1.308 (2) |
| V—O3 | 1.8155 (12) | C5—C4 | 1.456 (3) |
| V—O2 | 1.8421 (13) | C4—C3 | 1.386 (3) |
| V—O1 | 1.9300 (13) | C1—C2 | 1.341 (4) |
| V—N2 | 2.0992 (16) | C1—H6 | 0.9300 |
| V—O3$^{i}$ | 2.3950 (13) | C2—C3 | 1.425 (3) |
| S1—C1 | 1.695 (3) | C2—H4 | 0.9300 |
| S1—C4 | 1.715 (2) | C3—H5 | 0.9300 |
| O2—C9 | 1.321 (2) | C10—C15 | 1.387 (3) |
| O3—C16 | 1.426 (2) | C10—C11 | 1.404 (3) |
| O3—V$^{i}$ | 2.3950 (13) | C15—C14 | 1.373 (3) |
| N2—C6 | 1.315 (3) | C15—H12 | 0.9300 |
| N2—N1 | 1.399 (2) | C14—C13 | 1.380 (3) |
| N1—C5 | 1.295 (3) | C14—H11 | 0.9300 |
| C9—C8 | 1.359 (3) | C13—C12 | 1.370 (3) |
| C9—C10 | 1.477 (3) | C13—H10 | 0.9300 |
| C8—C6 | 1.424 (3) | C12—C11 | 1.372 (3) |
| C8—H7 | 0.9300 | C12—H9 | 0.9300 |
| C6—C7 | 1.494 (3) | C11—H8 | 0.9300 |
| C7—H2 | 0.9600 | C16—H15 | 0.9600 |
| C7—H3 | 0.9600 | C16—H13 | 0.9600 |
| C7—H1 | 0.9600 | C16—H14 | 0.9600 |
| | | | |
| O4—V—O3 | 103.06 (7) | N1—C5—C4 | 119.43 (17) |
| O4—V—O2 | 100.18 (7) | O1—C5—C4 | 117.45 (17) |
| O3—V—O2 | 103.99 (6) | C5—O1—V | 117.66 (12) |
| O4—V—O1 | 98.62 (7) | C3—C4—C5 | 126.90 (19) |
| O3—V—O1 | 90.23 (6) | C3—C4—S1 | 111.43 (15) |
| O2—V—O1 | 153.09 (7) | C5—C4—S1 | 121.67 (15) |
| O4—V—N2 | 97.68 (7) | C2—C1—S1 | 112.87 (18) |
| O3—V—N2 | 156.10 (6) | C2—C1—H6 | 123.6 |
| O2—V—N2 | 83.64 (6) | S1—C1—H6 | 123.6 |
| O1—V—N2 | 74.89 (6) | C1—C2—C3 | 113.0 (2) |
| O4—V—O3$^{i}$ | 174.44 (6) | C1—C2—H4 | 123.5 |
| O3—V—O3$^{i}$ | 71.92 (6) | C3—C2—H4 | 123.5 |
| O2—V—O3$^{i}$ | 79.07 (6) | C4—C3—C2 | 111.0 (2) |
| O1—V—O3$^{i}$ | 83.98 (5) | C4—C3—H5 | 124.5 |
| N2—V—O3$^{i}$ | 87.73 (5) | C2—C3—H5 | 124.5 |
| C1—S1—C4 | 91.68 (11) | C15—C10—C11 | 118.46 (18) |
| C9—O2—V | 133.45 (13) | C15—C10—C9 | 120.02 (17) |
| C16—O3—V | 124.60 (12) | C11—C10—C9 | 121.48 (17) |
| C16—O3—V$^{i}$ | 121.85 (11) | C14—C15—C10 | 120.71 (19) |

| | | | |
|---|---|---|---|
| V—O3—V$^{i}$ | 108.08 (6) | C14—C15—H12 | 119.6 |
| C6—N2—N1 | 115.69 (16) | C10—C15—H12 | 119.6 |
| C6—N2—V | 128.24 (13) | C15—C14—C13 | 120.2 (2) |
| N1—N2—V | 115.79 (12) | C15—C14—H11 | 119.9 |
| C5—N1—N2 | 107.93 (15) | C13—C14—H11 | 119.9 |
| O2—C9—C8 | 120.78 (18) | C12—C13—C14 | 119.8 (2) |
| O2—C9—C10 | 114.37 (16) | C12—C13—H10 | 120.1 |
| C8—C9—C10 | 124.84 (17) | C14—C13—H10 | 120.1 |
| C9—C8—C6 | 125.28 (18) | C13—C12—C11 | 120.78 (19) |
| C9—C8—H7 | 117.4 | C13—C12—H9 | 119.6 |
| C6—C8—H7 | 117.4 | C11—C12—H9 | 119.6 |
| N2—C6—C8 | 120.30 (17) | C12—C11—C10 | 120.02 (19) |
| N2—C6—C7 | 120.84 (19) | C12—C11—H8 | 120.0 |
| C8—C6—C7 | 118.85 (18) | C10—C11—H8 | 120.0 |
| C6—C7—H2 | 109.5 | O3—C16—H15 | 109.5 |
| C6—C7—H3 | 109.5 | O3—C16—H13 | 109.5 |
| H2—C7—H3 | 109.5 | H15—C16—H13 | 109.5 |
| C6—C7—H1 | 109.5 | O3—C16—H14 | 109.5 |
| H2—C7—H1 | 109.5 | H15—C16—H14 | 109.5 |
| H3—C7—H1 | 109.5 | H13—C16—H14 | 109.5 |
| N1—C5—O1 | 123.12 (17) | | |

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| O4—V—O2—C9 | −63.04 (19) | C9—C8—C6—N2 | 9.1 (3) |
| O3—V—O2—C9 | −169.38 (18) | C9—C8—C6—C7 | −171.7 (2) |
| O1—V—O2—C9 | 70.6 (2) | N2—N1—C5—O1 | −5.0 (2) |
| N2—V—O2—C9 | 33.66 (18) | N2—N1—C5—C4 | 174.88 (16) |
| O3$^{i}$—V—O2—C9 | 122.57 (19) | N1—C5—O1—V | 9.3 (2) |
| O4—V—O3—C16 | 28.39 (16) | C4—C5—O1—V | −170.54 (12) |
| O2—V—O3—C16 | 132.56 (15) | O4—V—O1—C5 | 88.96 (14) |
| O1—V—O3—C16 | −70.51 (15) | O3—V—O1—C5 | −167.79 (13) |
| N2—V—O3—C16 | −121.15 (18) | O2—V—O1—C5 | −45.0 (2) |
| O3$^{i}$—V—O3—C16 | −154.11 (17) | N2—V—O1—C5 | −6.73 (13) |
| O4—V—O3—V$^{i}$ | −177.50 (7) | O3$^{i}$—V—O1—C5 | −96.00 (13) |
| O2—V—O3—V$^{i}$ | −73.33 (7) | N1—C5—C4—C3 | −166.79 (19) |
| O1—V—O3—V$^{i}$ | 83.59 (6) | O1—C5—C4—C3 | 13.1 (3) |
| N2—V—O3—V$^{i}$ | 32.96 (16) | N1—C5—C4—S1 | 12.3 (3) |
| O3$^{i}$—V—O3—V$^{i}$ | 0.0 | O1—C5—C4—S1 | −167.85 (14) |
| O4—V—N2—C6 | 80.91 (18) | C1—S1—C4—C3 | −0.08 (16) |
| O3—V—N2—C6 | −128.97 (18) | C1—S1—C4—C5 | −179.28 (17) |
| O2—V—N2—C6 | −18.55 (17) | C4—S1—C1—C2 | 1.0 (2) |
| O1—V—N2—C6 | 177.82 (18) | S1—C1—C2—C3 | −1.6 (3) |
| O3$^{i}$—V—N2—C6 | −97.81 (17) | C5—C4—C3—C2 | 178.37 (19) |
| O4—V—N2—N1 | −92.68 (13) | S1—C4—C3—C2 | −0.8 (2) |
| O3—V—N2—N1 | 57.4 (2) | C1—C2—C3—C4 | 1.5 (3) |
| O2—V—N2—N1 | 167.86 (13) | O2—C9—C10—C15 | 16.0 (3) |
| O1—V—N2—N1 | 4.23 (12) | C8—C9—C10—C15 | −162.7 (2) |
| O3$^{i}$—V—N2—N1 | 88.60 (12) | O2—C9—C10—C11 | −161.71 (19) |
| C6—N2—N1—C5 | −175.49 (17) | C8—C9—C10—C11 | 19.6 (3) |

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| V—N2—N1—C5 | −1.07 (19) | C11—C10—C15—C14 | 0.0 (3) |
| V—O2—C9—C8 | −32.1 (3) | C9—C10—C15—C14 | −177.8 (2) |
| V—O2—C9—C10 | 149.16 (14) | C10—C15—C14—C13 | 0.7 (4) |
| O2—C9—C8—C6 | 2.4 (3) | C15—C14—C13—C12 | −0.2 (4) |
| C10—C9—C8—C6 | −179.02 (19) | C14—C13—C12—C11 | −1.0 (4) |
| N1—N2—C6—C8 | 177.40 (17) | C13—C12—C11—C10 | 1.7 (3) |
| V—N2—C6—C8 | 3.8 (3) | C15—C10—C11—C12 | −1.1 (3) |
| N1—N2—C6—C7 | −1.8 (3) | C9—C10—C11—C12 | 176.60 (19) |
| V—N2—C6—C7 | −175.38 (15) | | |

Symmetry code: (i) $-x$, $-y+2$, $-z+1$.