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# [3-Chloro-*N*′-(2-oxidonaphthalen-1-ylmethylidene)benzohydrazidato]-methanol(methanolato)oxidovanadium(V)

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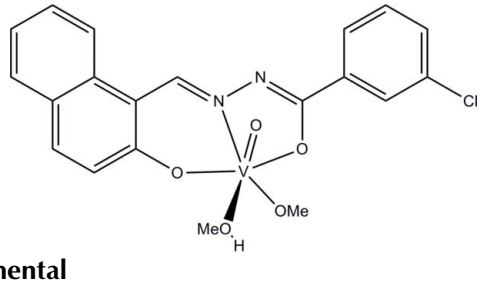
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.042; $wR$ factor = 0.109; data-to-parameter ratio = 16.3.

In the title complex, $[V(C_{18}H_{11}ClN_2O_2)(CH_3O)O(CH_3OH)]$, the $V^V$ ion is coordinated by a tridendate 3-chloro-*N*′-(2-oxidonaphthalen-1-ylmethylidene)benzohydrazidate ligand, one oxido ligand and by O atoms from a methanol and a methoxide ligand, forming a distorted octahedral geometry. The dihedral angle between the benzene ring and the naphthylene ring system is 6.4 (3)°. The deviation of the $V^V$ ion from the plane defined by the three donor atoms of the tridentate ligand and the methoxy O atom towards the oxido O atom is 0.323 (2) Å. In the crystal, pairs of intermolecular O—H···N hydrogen bonds form centrosymmetric dimers.

## Related literature

For background to hydrazones and their complexes, see: Seena *et al.* (2008); Bastos *et al.* (2008); Sarkar & Pal (2008); Nica *et al.* (2007). For the structure of a related oxidovanadium complex derived from *N*′-(5-bromo-2-hydroxybenzylidene)-2-chlorobenzohydrazide, see: Wang (2011). For other related oxidovanadium(V) complexes, see: Kurup *et al.* (2010); Rajak *et al.* (2000); Grüning *et al.* (1999); Mondal *et al.* (2009).




## Experimental

### Crystal data

$[V(C_{18}H_{11}ClN_2O_2)(CH_3O)O(CH_4O)]$
$M_r$ = 452.75
Monoclinic, $P2_1/n$
$a$ = 12.872 (3) Å
$b$ = 7.613 (2) Å
$c$ = 20.695 (3) Å
$\beta$ = 98.931 (3)°
$V$ = 2003.4 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.66 mm$^{-1}$
$T$ = 298 K
0.18 × 0.17 × 0.15 mm

### Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
$T_{min}$ = 0.890, $T_{max}$ = 0.907
13592 measured reflections
4368 independent reflections
3104 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.109
$S$ = 1.05
4368 reflections
268 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.43 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H4···N2$^{i}$ | 0.85 (1) | 1.99 (1) | 2.839 (3) | 178 (4) |

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5304).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, m1254 [ **doi:10.1107/S1600536811032703** ]

# [3-Chloro-*N*'-(2-oxidonaphthalen-1-ylmethylidene)benzohydrazidato]methanol(methanolato)oxidovanadium(V)

**F.-M. Wang**

## Comment

Hydrazone compounds and their oxovanadium complexes have received much attention due to their structural and biological properties (Seena *et al.*, 2008; Bastos *et al.*, 2008; Sarkar & Pal, 2008; Nica *et al.*, 2007). Recently, the author has reported a oxovanadium complex derived from N'-(5-bromo-2-hydroxybenzylidene)-2-chlorobenzohydrazide (Wang, 2011). In this paper, the crystal structure of the title compound is reported.

The $V^V$ ion in the title complex, Fig. 1, is six-coordinated by the phenolic O, imine N, and enolic O atoms of the hydrazone ligand, by one oxo O atom, and by two O atoms respectively from a methanol molecule and a methanolate ligand, forming a distorted octahedral geometry. The dihedral angle between the benzene ring and the naphthylene ring system of the hydrazone ligand is 6.4 (3)°. The deviation of the V atom from the plane defined by the three donor atoms of the hydrazone ligand and the methoxy O atom towards the oxo O atom is 0.323 (2) Å. The bond lengths and angles at the $V^V$ ion are comparable with those observed in similar oxovanadium(V) complexes (Kurup *et al.*, 2010; Rajak *et al.*, 2000; Grüning *et al.*, 1999; Mondal *et al.*, 2009). In the crystal, pairs of intermolecular O—H···N hydrogen bonds form centrosymmetric dimers (Fig. 2).

## Experimental

2-Hydroxy-1-naphthaldehyde (1 mmol, 0.17 g), 3-chlorobenzohydrazide 1 mmol, 0.17 g), and $VO(acac)_2$ (1 mmol, 0.26 g) were mixed in methanol (30 ml). The mixture was boiled under reflux for 2 h, then cooled to room temperature. Brown block-like single crystals, suitable for X-ray diffraction, were formed after slow evaporation of the solution in air for a few days.

## Refinement

Atom H4 was located from a difference Fourier map and refined isotropically. The O4—H4 distance was restrained to 0.85 (1) Å. The remaining hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.96 Å, and with $U_{iso}$(H) set at 1.2$U_{eq}$(C) and 1.5$U_{eq}$($C_{methyl}$).

## Figures

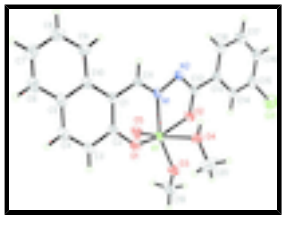

Fig. 1. The molecular structure of the title compound with displacement ellipsoids are drawn at the 30% probability level.

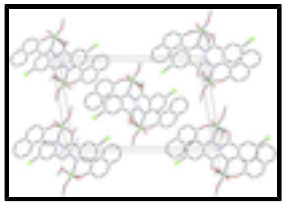

Fig. 2. Part of the crystal structure with hydrogen bonds shown as dashed lines.

**[3-Chloro-*N*'-(2-oxidonaphthalen-1- ylmethylidene)benzohydrazidato]methanol(methanolato)oxidovanadium(V)**

*Crystal data*

| | |
|---|---|
| $[V(C_{18}H_{11}ClN_2O_2)(CH_3O)O(CH_4O)]$ | $F(000) = 928$ |
| $M_r = 452.75$ | $D_x = 1.501$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2yn | Cell parameters from 3491 reflections |
| $a = 12.872$ (3) Å | $\theta = 2.8–26.0°$ |
| $b = 7.613$ (2) Å | $\mu = 0.66$ mm$^{-1}$ |
| $c = 20.695$ (3) Å | $T = 298$ K |
| $\beta = 98.931$ (3)° | Block, brown |
| $V = 2003.4$ (8) Å$^3$ | 0.18 × 0.17 × 0.15 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD diffractometer | 4368 independent reflections |
| Radiation source: fine-focus sealed tube | 3104 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.036$ |
| ω scan | $\theta_{max} = 27.0°$, $\theta_{min} = 2.9°$ |
| Absorption correction: multi-scan *SADABS* (Sheldrick, 1996) | $h = -14\rightarrow16$ |
| $T_{min} = 0.890$, $T_{max} = 0.907$ | $k = -9\rightarrow9$ |
| 13592 measured reflections | $l = -26\rightarrow26$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.109$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 0.9229P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 4368 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 268 parameters | $\Delta\rho_{max} = 0.34$ e Å$^{-3}$ |
| 1 restraint | $\Delta\rho_{min} = -0.43$ 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.

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| V1 | 0.26454 (3) | 0.08667 (6) | 0.99698 (2) | 0.03892 (14) |
| Cl1 | 0.15025 (8) | 0.45711 (15) | 1.28761 (4) | 0.0857 (3) |
| N1 | 0.10581 (15) | 0.1236 (2) | 0.95334 (9) | 0.0317 (4) |
| N2 | 0.04044 (15) | 0.2021 (3) | 0.99338 (9) | 0.0338 (5) |
| O1 | 0.26311 (14) | −0.0734 (3) | 0.92934 (8) | 0.0472 (5) |
| O2 | 0.19838 (13) | 0.2083 (2) | 1.06222 (8) | 0.0417 (4) |
| O3 | 0.37183 (13) | 0.0107 (3) | 1.05311 (8) | 0.0467 (5) |
| O4 | 0.17893 (14) | −0.1470 (3) | 1.04327 (9) | 0.0469 (5) |
| O5 | 0.31027 (15) | 0.2518 (3) | 0.96509 (10) | 0.0601 (5) |
| C1 | 0.11838 (18) | 0.0029 (3) | 0.84704 (11) | 0.0328 (5) |
| C2 | 0.21637 (19) | −0.0746 (3) | 0.86749 (12) | 0.0367 (6) |
| C3 | 0.2684 (2) | −0.1682 (4) | 0.82235 (13) | 0.0438 (6) |
| H3 | 0.3329 | −0.2215 | 0.8365 | 0.053* |
| C4 | 0.2240 (2) | −0.1799 (4) | 0.75880 (13) | 0.0451 (7) |
| H4A | 0.2592 | −0.2412 | 0.7299 | 0.054* |
| C5 | 0.1258 (2) | −0.1019 (3) | 0.73489 (12) | 0.0418 (6) |
| C6 | 0.0817 (2) | −0.1125 (4) | 0.66811 (13) | 0.0547 (8) |
| H6 | 0.1183 | −0.1709 | 0.6392 | 0.066* |
| C7 | −0.0130 (3) | −0.0392 (5) | 0.64528 (15) | 0.0657 (9) |
| H7 | −0.0405 | −0.0465 | 0.6011 | 0.079* |
| C8 | −0.0688 (2) | 0.0469 (4) | 0.68830 (15) | 0.0626 (9) |
| H8 | −0.1343 | 0.0951 | 0.6727 | 0.075* |
| C9 | −0.0285 (2) | 0.0615 (4) | 0.75334 (13) | 0.0476 (7) |
| H9 | −0.0670 | 0.1207 | 0.7810 | 0.057* |
| C10 | 0.07055 (19) | −0.0116 (3) | 0.77942 (11) | 0.0360 (6) |
| C11 | 0.06312 (18) | 0.0867 (3) | 0.89423 (11) | 0.0331 (5) |
| H11 | −0.0072 | 0.1158 | 0.8813 | 0.040* |
| C12 | 0.09845 (18) | 0.2435 (3) | 1.04907 (11) | 0.0332 (5) |
| C13 | 0.05144 (19) | 0.3322 (3) | 1.10122 (11) | 0.0345 (5) |
| C14 | 0.1116 (2) | 0.3473 (3) | 1.16256 (12) | 0.0403 (6) |
| H14 | 0.1790 | 0.2999 | 1.1703 | 0.048* |
| C15 | 0.0718 (2) | 0.4319 (4) | 1.21188 (13) | 0.0485 (7) |
| C16 | −0.0294 (2) | 0.4999 (4) | 1.20174 (14) | 0.0525 (7) |

| | | | | |
|---|---|---|---|---|
| H16 | −0.0565 | 0.5546 | 1.2357 | 0.063* |
| C17 | −0.0890 (2) | 0.4853 (4) | 1.14100 (14) | 0.0506 (7) |
| H17 | −0.1569 | 0.5308 | 1.1339 | 0.061* |
| C18 | −0.0496 (2) | 0.4041 (3) | 1.09024 (13) | 0.0424 (6) |
| H18 | −0.0902 | 0.3972 | 1.0490 | 0.051* |
| C19 | 0.4735 (2) | 0.0765 (5) | 1.07551 (15) | 0.0683 (10) |
| H19A | 0.4918 | 0.1617 | 1.0450 | 0.102* |
| H19B | 0.5232 | −0.0183 | 1.0793 | 0.102* |
| H19C | 0.4746 | 0.1308 | 1.1175 | 0.102* |
| C20 | 0.2289 (3) | −0.3005 (5) | 1.0690 (2) | 0.0865 (12) |
| H20A | 0.2443 | −0.3737 | 1.0340 | 0.130* |
| H20B | 0.1835 | −0.3626 | 1.0939 | 0.130* |
| H20C | 0.2932 | −0.2706 | 1.0970 | 0.130* |
| H4 | 0.1136 (9) | −0.162 (5) | 1.0318 (16) | 0.086 (12)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| V1 | 0.0281 (2) | 0.0508 (3) | 0.0397 (2) | 0.0009 (2) | 0.01096 (17) | 0.0007 (2) |
| Cl1 | 0.0987 (7) | 0.1131 (8) | 0.0431 (4) | 0.0125 (6) | 0.0045 (4) | −0.0194 (5) |
| N1 | 0.0312 (10) | 0.0324 (11) | 0.0345 (10) | 0.0022 (9) | 0.0144 (8) | 0.0005 (8) |
| N2 | 0.0319 (11) | 0.0376 (12) | 0.0348 (10) | 0.0026 (9) | 0.0140 (9) | −0.0003 (9) |
| O1 | 0.0402 (10) | 0.0614 (12) | 0.0407 (10) | 0.0165 (9) | 0.0080 (8) | −0.0048 (9) |
| O2 | 0.0298 (9) | 0.0546 (12) | 0.0417 (9) | −0.0012 (8) | 0.0091 (7) | −0.0083 (8) |
| O3 | 0.0282 (9) | 0.0654 (13) | 0.0460 (10) | −0.0008 (9) | 0.0045 (8) | −0.0069 (9) |
| O4 | 0.0343 (11) | 0.0462 (11) | 0.0585 (12) | −0.0021 (9) | 0.0016 (9) | 0.0122 (9) |
| O5 | 0.0502 (12) | 0.0660 (14) | 0.0703 (13) | −0.0063 (11) | 0.0291 (10) | 0.0096 (11) |
| C1 | 0.0322 (13) | 0.0325 (13) | 0.0359 (12) | −0.0026 (11) | 0.0124 (10) | −0.0003 (10) |
| C2 | 0.0361 (13) | 0.0364 (14) | 0.0400 (13) | −0.0006 (11) | 0.0131 (11) | −0.0003 (11) |
| C3 | 0.0336 (14) | 0.0470 (16) | 0.0535 (16) | 0.0038 (12) | 0.0153 (12) | −0.0045 (13) |
| C4 | 0.0449 (16) | 0.0456 (17) | 0.0495 (16) | −0.0048 (13) | 0.0225 (13) | −0.0116 (13) |
| C5 | 0.0441 (15) | 0.0394 (15) | 0.0447 (14) | −0.0127 (12) | 0.0154 (12) | −0.0065 (12) |
| C6 | 0.0572 (19) | 0.064 (2) | 0.0453 (15) | −0.0155 (16) | 0.0163 (14) | −0.0188 (14) |
| C7 | 0.061 (2) | 0.087 (3) | 0.0462 (17) | −0.0128 (19) | −0.0015 (15) | −0.0195 (17) |
| C8 | 0.0508 (18) | 0.079 (2) | 0.0538 (18) | 0.0010 (16) | −0.0059 (15) | −0.0124 (16) |
| C9 | 0.0415 (15) | 0.0559 (18) | 0.0446 (15) | 0.0002 (13) | 0.0039 (12) | −0.0104 (13) |
| C10 | 0.0365 (14) | 0.0342 (14) | 0.0390 (13) | −0.0078 (11) | 0.0113 (11) | −0.0027 (11) |
| C11 | 0.0285 (12) | 0.0347 (13) | 0.0372 (12) | −0.0003 (11) | 0.0082 (10) | 0.0046 (11) |
| C12 | 0.0323 (13) | 0.0315 (13) | 0.0382 (12) | −0.0042 (11) | 0.0129 (10) | 0.0017 (10) |
| C13 | 0.0358 (13) | 0.0300 (13) | 0.0406 (13) | −0.0053 (11) | 0.0142 (11) | −0.0005 (10) |
| C14 | 0.0394 (14) | 0.0429 (15) | 0.0408 (14) | −0.0016 (12) | 0.0134 (11) | −0.0005 (11) |
| C15 | 0.0587 (18) | 0.0502 (18) | 0.0392 (14) | −0.0060 (15) | 0.0163 (13) | −0.0045 (12) |
| C16 | 0.063 (2) | 0.0482 (18) | 0.0529 (17) | −0.0029 (15) | 0.0306 (15) | −0.0096 (14) |
| C17 | 0.0446 (16) | 0.0410 (16) | 0.071 (2) | 0.0002 (13) | 0.0229 (15) | −0.0087 (14) |
| C18 | 0.0435 (15) | 0.0377 (15) | 0.0474 (15) | −0.0021 (12) | 0.0111 (12) | −0.0042 (12) |
| C19 | 0.0375 (16) | 0.108 (3) | 0.0586 (19) | −0.0146 (17) | 0.0047 (14) | −0.0152 (19) |
| C20 | 0.070 (2) | 0.065 (2) | 0.111 (3) | −0.0051 (19) | −0.026 (2) | 0.032 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| V1—O5 | 1.576 (2) | C6—H6 | 0.9300 |
| V1—O3 | 1.7587 (18) | C7—C8 | 1.392 (4) |
| V1—O1 | 1.8539 (18) | C7—H7 | 0.9300 |
| V1—O2 | 1.9398 (17) | C8—C9 | 1.370 (4) |
| V1—N1 | 2.120 (2) | C8—H8 | 0.9300 |
| V1—O4 | 2.371 (2) | C9—C10 | 1.419 (4) |
| Cl1—C15 | 1.738 (3) | C9—H9 | 0.9300 |
| N1—C11 | 1.292 (3) | C11—H11 | 0.9300 |
| N1—N2 | 1.403 (3) | C12—C13 | 1.480 (3) |
| N2—C12 | 1.311 (3) | C13—C14 | 1.385 (3) |
| O1—C2 | 1.327 (3) | C13—C18 | 1.397 (4) |
| O2—C12 | 1.301 (3) | C14—C15 | 1.371 (4) |
| O3—C19 | 1.410 (3) | C14—H14 | 0.9300 |
| O4—C20 | 1.400 (4) | C15—C16 | 1.387 (4) |
| O4—H4 | 0.845 (10) | C16—C17 | 1.372 (4) |
| C1—C2 | 1.397 (3) | C16—H16 | 0.9300 |
| C1—C10 | 1.443 (3) | C17—C18 | 1.382 (4) |
| C1—C11 | 1.443 (3) | C17—H17 | 0.9300 |
| C2—C3 | 1.423 (3) | C18—H18 | 0.9300 |
| C3—C4 | 1.353 (4) | C19—H19A | 0.9600 |
| C3—H3 | 0.9300 | C19—H19B | 0.9600 |
| C4—C5 | 1.415 (4) | C19—H19C | 0.9600 |
| C4—H4A | 0.9300 | C20—H20A | 0.9600 |
| C5—C6 | 1.413 (4) | C20—H20B | 0.9600 |
| C5—C10 | 1.425 (3) | C20—H20C | 0.9600 |
| C6—C7 | 1.357 (4) | | |
| O5—V1—O3 | 103.46 (10) | C9—C8—C7 | 120.8 (3) |
| O5—V1—O1 | 99.70 (10) | C9—C8—H8 | 119.6 |
| O3—V1—O1 | 101.38 (8) | C7—C8—H8 | 119.6 |
| O5—V1—O2 | 98.26 (9) | C8—C9—C10 | 121.5 (3) |
| O3—V1—O2 | 94.70 (8) | C8—C9—H9 | 119.2 |
| O1—V1—O2 | 152.31 (8) | C10—C9—H9 | 119.2 |
| O5—V1—N1 | 96.54 (9) | C9—C10—C5 | 116.9 (2) |
| O3—V1—N1 | 158.57 (8) | C9—C10—C1 | 124.2 (2) |
| O1—V1—N1 | 82.51 (8) | C5—C10—C1 | 118.9 (2) |
| O2—V1—N1 | 74.64 (7) | N1—C11—C1 | 123.7 (2) |
| O5—V1—O4 | 174.17 (9) | N1—C11—H11 | 118.1 |
| O3—V1—O4 | 81.55 (8) | C1—C11—H11 | 118.1 |
| O1—V1—O4 | 82.03 (8) | O2—C12—N2 | 123.0 (2) |
| O2—V1—O4 | 78.18 (8) | O2—C12—C13 | 116.4 (2) |
| N1—V1—O4 | 78.11 (7) | N2—C12—C13 | 120.6 (2) |
| C11—N1—N2 | 116.49 (19) | C14—C13—C18 | 119.4 (2) |
| C11—N1—V1 | 127.92 (16) | C14—C13—C12 | 118.2 (2) |
| N2—N1—V1 | 115.56 (14) | C18—C13—C12 | 122.4 (2) |
| C12—N2—N1 | 108.04 (19) | C15—C14—C13 | 120.1 (3) |
| C2—O1—V1 | 133.04 (16) | C15—C14—H14 | 120.0 |

| | | | |
|---|---|---|---|
| C12—O2—V1 | 118.64 (15) | C13—C14—H14 | 120.0 |
| C19—O3—V1 | 133.9 (2) | C14—C15—C16 | 120.8 (3) |
| C20—O4—V1 | 124.4 (2) | C14—C15—Cl1 | 119.5 (2) |
| C20—O4—H4 | 112 (3) | C16—C15—Cl1 | 119.7 (2) |
| V1—O4—H4 | 119 (2) | C17—C16—C15 | 119.2 (3) |
| C2—C1—C10 | 119.4 (2) | C17—C16—H16 | 120.4 |
| C2—C1—C11 | 119.9 (2) | C15—C16—H16 | 120.4 |
| C10—C1—C11 | 120.6 (2) | C16—C17—C18 | 120.9 (3) |
| O1—C2—C1 | 122.8 (2) | C16—C17—H17 | 119.5 |
| O1—C2—C3 | 116.6 (2) | C18—C17—H17 | 119.5 |
| C1—C2—C3 | 120.5 (2) | C17—C18—C13 | 119.6 (3) |
| C4—C3—C2 | 120.1 (2) | C17—C18—H18 | 120.2 |
| C4—C3—H3 | 120.0 | C13—C18—H18 | 120.2 |
| C2—C3—H3 | 120.0 | O3—C19—H19A | 109.5 |
| C3—C4—C5 | 122.1 (2) | O3—C19—H19B | 109.5 |
| C3—C4—H4A | 118.9 | H19A—C19—H19B | 109.5 |
| C5—C4—H4A | 118.9 | O3—C19—H19C | 109.5 |
| C6—C5—C4 | 121.3 (2) | H19A—C19—H19C | 109.5 |
| C6—C5—C10 | 119.7 (3) | H19B—C19—H19C | 109.5 |
| C4—C5—C10 | 119.0 (2) | O4—C20—H20A | 109.5 |
| C7—C6—C5 | 121.3 (3) | O4—C20—H20B | 109.5 |
| C7—C6—H6 | 119.3 | H20A—C20—H20B | 109.5 |
| C5—C6—H6 | 119.3 | O4—C20—H20C | 109.5 |
| C6—C7—C8 | 119.7 (3) | H20A—C20—H20C | 109.5 |
| C6—C7—H7 | 120.1 | H20B—C20—H20C | 109.5 |
| C8—C7—H7 | 120.1 | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H4···N2$^{i}$ | 0.85 (1) | 1.99 (1) | 2.839 (3) | 178 (4) |

Symmetry codes: (i) −*x*, −*y*, −*z*+2.

**Fig. 1**

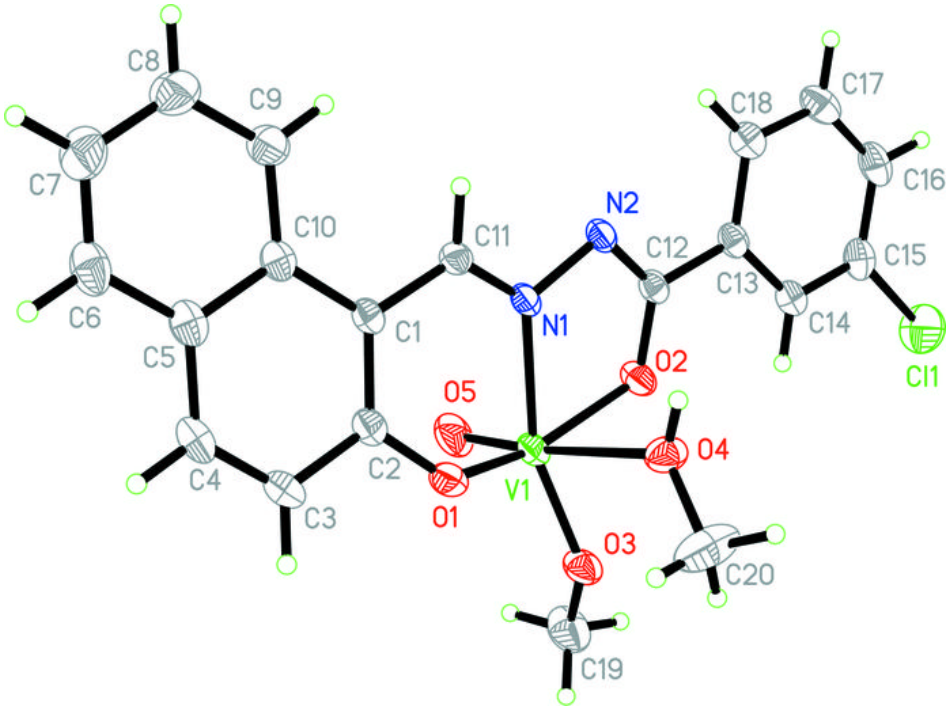
C8
C9
C7
C10
C11
N2
C12
C18
C17
C16
C15
C13
C14
Cl1
C6
C5
C1
N1
O2
O5
O4
C4
C2
V1
C3
O1
O3
C20
C19

**Fig. 2**