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# [*N*′-(3-Ethoxy-2-oxidobenzylidene-$\kappa O^2$)-4-methylbenzohydrazidato-$\kappa^2 O,N'$]-(methanolato-$\kappa O$)oxidovanadium(V)

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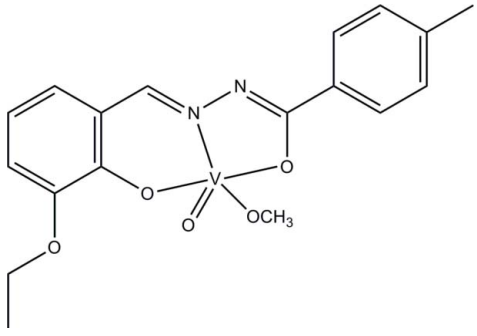
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.045; $wR$ factor = 0.110; data-to-parameter ratio = 17.0.

The title oxidovanadium(V) complex, $[V(C_{17}H_{16}N_2O_3)(CH_3O)O]$, was obtained by the reaction of 3-ethoxy-2-hydroxybenzaldehyde, 4-methylbenzohydrazide and vanadyl sulfate in methanol. The $V^V$ atom is coordinated by the *O*,*N*,*O*′-tridentate Schiff base ligand, one methanolate O atom and one oxide O atom, forming a distorted $VO_4N$ square-pyramidal coordination geometry. The oxide O atom lies at the apex of the square pyramid and the N atom of the ligand and the methanolate O atom are *trans*. The dihedral angle between the benzene rings of the ligand is 1.8 (3)°.

## Related literature

For background to Schiff base complexes, see: Wang (2009); Wang & Ye (2011). For similar vanadium(V) complexes, see: Wang *et al.* (2011); Deng *et al.* (2005); Gao *et al.* (2005); Huo *et al.* (2004).




## Experimental

### Crystal data

$[V(C_{17}H_{16}N_2O_3)(CH_3O)O]$ $M_r$ = 394.29
Monoclinic, $P2_1/c$
$a$ = 7.6954 (16) Å
$b$ = 28.345 (3) Å
$c$ = 8.3877 (18) Å
$\beta$ = 105.175 (2)°
$V$ = 1765.8 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.59 mm$^{-1}$
$T$ = 298 K
0.30 × 0.27 × 0.27 mm

### Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.842, $T_{max}$ = 0.856
14022 measured reflections
4044 independent reflections
2986 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.110
$S$ = 1.05
4044 reflections
238 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.30 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| V1—O5 | 1.5813 (17) | V1—O3 | 1.9170 (16) |
| V1—O4 | 1.7499 (17) | V1—N1 | 2.1031 (19) |
| V1—O1 | 1.8326 (16) | | |

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: HB6443).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, m1538 [ **doi:10.1107/S1600536811041547** ]

# [*N*'-(3-Ethoxy-2-oxidobenzylidene-$\kappa O^2$)-4-methylbenzohydrazidato-$\kappa^2 O,N'$](methanolato-$\kappa O$)oxidovanadium(V)

**C.-Y. Wang, X. Wu, F. Cao and C.-J. Yuan**

## Comment

As part of our investigations into new Schiff base complexes and urease inhibition (Wang & Ye, 2011; Wang, 2009), we have synthesized the title compound, (I), a new mononuclear oxovanadium(V) complex, Fig. 1. The V atom in the complex is five-coordinated by the O,N,O-tridentate Schiff base ligand, one methanolate O atom, and one oxide O atom, forming a distorted square-pyramidal geometry. The oxide O atom lies on the apical position of the square-pyramidal geometry. The dihedral angle between the two benzene rings is 1.8 (3)°. The V–O and V–N bond lengths (Table 1) are typical and are comparable with those observed in other similar vanadium complexes (Wang *et al.*, 2011; Deng *et al.*, 2005; Gao *et al.*, 2005; Huo *et al.*, 2004).

## Experimental

3-Ethoxy-2-hydroxybenzaldehyde (1.0 mmol, 0.17 g), 4-methylbenzohydrazide (1.0 mmol, 0.15 g), and vanadyl sulfate (1.0 mmol, 0.16 g) were dissolved in methanol (30 ml). The mixture was stirred at room temperature for 10 min to give a clear brown solution. After keeping the solution in air for a week, brown block-shaped crystals were formed at the bottom of the vessel.

## Refinement

Hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{iso}$(H) set at 1.2 or 1.5$U_{eq}$(C).

## Figures

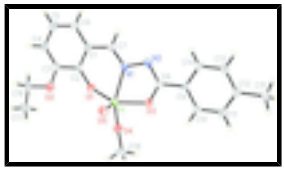

Fig. 1. The molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level.

## [*N*'-(3-Ethoxy-2-oxidobenzylidene-κ$O^2$)-4- methylbenzohydrazidato-$\kappa^2 O,N'$](methanolato-κ*O*)oxidovanadium(V)

*Crystal data*

| | |
|---|---|
| $[V(C_{17}H_{16}N_2O_3)(CH_3O)O]$ | $F(000) = 816$ |
| $M_r = 394.29$ | $D_x = 1.483$ Mg m$^{-3}$ |

| | |
|---|---|
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 3023 reflections |
| $a = 7.6954$ (16) Å | $\theta = 2.6–25.0°$ |
| $b = 28.345$ (3) Å | $\mu = 0.59$ mm$^{-1}$ |
| $c = 8.3877$ (18) Å | $T = 298$ K |
| $\beta = 105.175$ (2)° | Block, brown |
| $V = 1765.8$ (6) Å$^3$ | 0.30 × 0.27 × 0.27 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD diffractometer | 4044 independent reflections |
| Radiation source: fine-focus sealed tube | 2986 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.039$ |
| ω scans | $\theta_{max} = 27.5°$, $\theta_{min} = 2.6°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -9\rightarrow9$ |
| $T_{min} = 0.842$, $T_{max} = 0.856$ | $k = -36\rightarrow35$ |
| 14022 measured reflections | $l = -10\rightarrow10$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.045$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.110$ | H-atom parameters constrained |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.4204P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 4044 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 238 parameters | $\Delta\rho_{max} = 0.27$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.30$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| V1 | 0.23672 (5) | 0.414915 (13) | 0.47578 (5) | 0.03413 (14) |
| N1 | 0.1850 (2) | 0.34208 (6) | 0.4771 (2) | 0.0333 (4) |
| N2 | 0.0915 (3) | 0.32243 (7) | 0.3264 (2) | 0.0386 (5) |
| O1 | 0.3948 (2) | 0.40199 (5) | 0.67570 (19) | 0.0407 (4) |
| O2 | 0.5797 (2) | 0.42530 (6) | 0.9805 (2) | 0.0477 (5) |
| O3 | 0.1583 (2) | 0.39594 (6) | 0.24884 (19) | 0.0411 (4) |
| O4 | 0.3495 (2) | 0.46251 (6) | 0.4152 (2) | 0.0478 (4) |
| O5 | 0.0567 (2) | 0.43456 (6) | 0.5082 (2) | 0.0479 (4) |
| C1 | 0.3177 (3) | 0.32665 (8) | 0.7653 (3) | 0.0342 (5) |
| C2 | 0.4022 (3) | 0.37085 (8) | 0.7972 (3) | 0.0340 (5) |
| C3 | 0.5005 (3) | 0.38212 (9) | 0.9597 (3) | 0.0386 (6) |
| C4 | 0.5096 (3) | 0.34910 (10) | 1.0833 (3) | 0.0466 (6) |
| H4 | 0.5724 | 0.3564 | 1.1910 | 0.056* |
| C5 | 0.4279 (3) | 0.30551 (10) | 1.0504 (3) | 0.0498 (7) |
| H5 | 0.4376 | 0.2839 | 1.1358 | 0.060* |
| C6 | 0.3330 (3) | 0.29378 (9) | 0.8939 (3) | 0.0422 (6) |
| H6 | 0.2789 | 0.2643 | 0.8726 | 0.051* |
| C7 | 0.2177 (3) | 0.31382 (8) | 0.6028 (3) | 0.0350 (5) |
| H7 | 0.1731 | 0.2832 | 0.5860 | 0.042* |
| C8 | 0.0825 (3) | 0.35451 (8) | 0.2130 (3) | 0.0336 (5) |
| C9 | −0.0137 (3) | 0.34495 (8) | 0.0398 (3) | 0.0324 (5) |
| C10 | −0.0244 (3) | 0.37956 (9) | −0.0791 (3) | 0.0411 (6) |
| H10 | 0.0317 | 0.4085 | −0.0499 | 0.049* |
| C11 | −0.1182 (3) | 0.37113 (9) | −0.2405 (3) | 0.0449 (6) |
| H11 | −0.1248 | 0.3947 | −0.3188 | 0.054* |
| C12 | −0.2024 (3) | 0.32857 (9) | −0.2889 (3) | 0.0388 (6) |
| C13 | −0.1894 (3) | 0.29402 (9) | −0.1695 (3) | 0.0439 (6) |
| H13 | −0.2440 | 0.2649 | −0.1994 | 0.053* |
| C14 | −0.0972 (3) | 0.30194 (8) | −0.0072 (3) | 0.0393 (6) |
| H14 | −0.0911 | 0.2783 | 0.0710 | 0.047* |
| C15 | −0.3043 (4) | 0.32044 (11) | −0.4656 (3) | 0.0559 (7) |
| H15A | −0.3865 | 0.3461 | −0.5028 | 0.084* |
| H15B | −0.3704 | 0.2914 | −0.4740 | 0.084* |
| H15C | −0.2212 | 0.3186 | −0.5331 | 0.084* |
| C16 | 0.6757 (4) | 0.43846 (10) | 1.1461 (3) | 0.0546 (7) |
| H16A | 0.7681 | 0.4153 | 1.1917 | 0.065* |
| H16B | 0.5935 | 0.4399 | 1.2161 | 0.065* |
| C17 | 0.7590 (4) | 0.48552 (11) | 1.1390 (4) | 0.0727 (10) |
| H17A | 0.8465 | 0.4833 | 1.0761 | 0.109* |
| H17B | 0.8169 | 0.4959 | 1.2490 | 0.109* |
| H17C | 0.6674 | 0.5078 | 1.0873 | 0.109* |
| C18 | 0.2882 (4) | 0.50506 (11) | 0.3339 (4) | 0.0795 (11) |
| H18A | 0.1982 | 0.4985 | 0.2333 | 0.119* |
| H18B | 0.3873 | 0.5213 | 0.3090 | 0.119* |
| H18C | 0.2373 | 0.5244 | 0.4040 | 0.119* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| V1 | 0.0416 (2) | 0.0292 (2) | 0.0292 (2) | −0.00241 (17) | 0.00511 (16) | 0.00033 (17) |
| N1 | 0.0382 (10) | 0.0303 (10) | 0.0294 (10) | −0.0005 (8) | 0.0050 (8) | −0.0002 (8) |
| N2 | 0.0492 (12) | 0.0339 (11) | 0.0280 (10) | −0.0048 (9) | 0.0018 (8) | −0.0042 (8) |
| O1 | 0.0486 (10) | 0.0349 (9) | 0.0324 (9) | −0.0063 (7) | −0.0004 (7) | 0.0007 (7) |
| O2 | 0.0515 (10) | 0.0465 (11) | 0.0352 (10) | 0.0005 (8) | −0.0063 (8) | −0.0065 (8) |
| O3 | 0.0569 (10) | 0.0346 (9) | 0.0302 (9) | −0.0100 (8) | 0.0086 (7) | −0.0009 (7) |
| O4 | 0.0544 (10) | 0.0414 (10) | 0.0427 (10) | −0.0136 (8) | 0.0042 (8) | 0.0062 (8) |
| O5 | 0.0524 (10) | 0.0444 (10) | 0.0480 (11) | 0.0074 (8) | 0.0151 (8) | 0.0006 (8) |
| C1 | 0.0334 (11) | 0.0370 (13) | 0.0315 (12) | 0.0051 (10) | 0.0071 (9) | 0.0009 (10) |
| C2 | 0.0355 (12) | 0.0344 (12) | 0.0304 (12) | 0.0080 (10) | 0.0057 (9) | 0.0025 (10) |
| C3 | 0.0381 (12) | 0.0412 (14) | 0.0339 (13) | 0.0079 (10) | 0.0049 (10) | −0.0038 (10) |
| C4 | 0.0488 (14) | 0.0608 (18) | 0.0259 (13) | 0.0095 (13) | 0.0021 (10) | 0.0025 (12) |
| C5 | 0.0573 (16) | 0.0549 (17) | 0.0357 (14) | 0.0058 (13) | 0.0093 (12) | 0.0144 (13) |
| C6 | 0.0450 (13) | 0.0436 (15) | 0.0381 (14) | 0.0015 (11) | 0.0110 (11) | 0.0085 (11) |
| C7 | 0.0397 (12) | 0.0291 (12) | 0.0353 (13) | −0.0004 (9) | 0.0084 (10) | 0.0010 (10) |
| C8 | 0.0378 (12) | 0.0325 (12) | 0.0309 (12) | −0.0002 (10) | 0.0094 (9) | −0.0009 (10) |
| C9 | 0.0358 (12) | 0.0339 (12) | 0.0277 (12) | 0.0035 (9) | 0.0086 (9) | −0.0019 (10) |
| C10 | 0.0516 (14) | 0.0368 (14) | 0.0353 (13) | −0.0018 (11) | 0.0124 (11) | −0.0004 (11) |
| C11 | 0.0546 (15) | 0.0486 (15) | 0.0337 (14) | 0.0082 (12) | 0.0157 (11) | 0.0093 (12) |
| C12 | 0.0367 (12) | 0.0491 (15) | 0.0304 (13) | 0.0055 (11) | 0.0083 (10) | −0.0018 (11) |
| C13 | 0.0478 (14) | 0.0448 (15) | 0.0359 (14) | −0.0070 (11) | 0.0054 (11) | −0.0056 (11) |
| C14 | 0.0466 (13) | 0.0382 (14) | 0.0306 (13) | −0.0010 (11) | 0.0058 (10) | 0.0024 (10) |
| C15 | 0.0592 (16) | 0.071 (2) | 0.0323 (14) | 0.0095 (15) | 0.0031 (12) | −0.0006 (14) |
| C16 | 0.0515 (15) | 0.0630 (18) | 0.0385 (15) | 0.0086 (14) | −0.0072 (12) | −0.0153 (13) |
| C17 | 0.071 (2) | 0.062 (2) | 0.067 (2) | −0.0001 (16) | −0.0148 (16) | −0.0230 (17) |
| C18 | 0.069 (2) | 0.062 (2) | 0.092 (3) | −0.0136 (16) | −0.0071 (18) | 0.0393 (18) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| V1—O5 | 1.5813 (17) | C8—C9 | 1.473 (3) |
| V1—O4 | 1.7499 (17) | C9—C10 | 1.386 (3) |
| V1—O1 | 1.8326 (16) | C9—C14 | 1.386 (3) |
| V1—O3 | 1.9170 (16) | C10—C11 | 1.378 (3) |
| V1—N1 | 2.1031 (19) | C10—H10 | 0.9300 |
| N1—C7 | 1.295 (3) | C11—C12 | 1.380 (3) |
| N1—N2 | 1.396 (2) | C11—H11 | 0.9300 |
| N2—C8 | 1.305 (3) | C12—C13 | 1.385 (3) |
| O1—C2 | 1.338 (3) | C12—C15 | 1.502 (3) |
| O2—C3 | 1.358 (3) | C13—C14 | 1.379 (3) |
| O2—C16 | 1.441 (3) | C13—H13 | 0.9300 |
| O3—C8 | 1.311 (3) | C14—H14 | 0.9300 |
| O4—C18 | 1.405 (3) | C15—H15A | 0.9600 |
| C1—C2 | 1.405 (3) | C15—H15B | 0.9600 |
| C1—C6 | 1.407 (3) | C15—H15C | 0.9600 |
| C1—C7 | 1.426 (3) | C16—C17 | 1.488 (4) |

| | | | |
|---|---|---|---|
| C2—C3 | 1.412 (3) | C16—H16A | 0.9700 |
| C3—C4 | 1.384 (3) | C16—H16B | 0.9700 |
| C4—C5 | 1.381 (4) | C17—H17A | 0.9600 |
| C4—H4 | 0.9300 | C17—H17B | 0.9600 |
| C5—C6 | 1.366 (3) | C17—H17C | 0.9600 |
| C5—H5 | 0.9300 | C18—H18A | 0.9600 |
| C6—H6 | 0.9300 | C18—H18B | 0.9600 |
| C7—H7 | 0.9300 | C18—H18C | 0.9600 |
| O5—V1—O4 | 107.58 (9) | C10—C9—C14 | 118.8 (2) |
| O5—V1—O1 | 108.34 (9) | C10—C9—C8 | 120.0 (2) |
| O4—V1—O1 | 99.14 (8) | C14—C9—C8 | 121.2 (2) |
| O5—V1—O3 | 101.98 (8) | C11—C10—C9 | 120.1 (2) |
| O4—V1—O3 | 88.79 (7) | C11—C10—H10 | 119.9 |
| O1—V1—O3 | 144.43 (8) | C9—C10—H10 | 119.9 |
| O5—V1—N1 | 99.74 (8) | C10—C11—C12 | 121.7 (2) |
| O4—V1—N1 | 150.14 (8) | C10—C11—H11 | 119.1 |
| O1—V1—N1 | 83.11 (7) | C12—C11—H11 | 119.1 |
| O3—V1—N1 | 73.70 (7) | C11—C12—C13 | 117.8 (2) |
| C7—N1—N2 | 115.75 (19) | C11—C12—C15 | 120.6 (2) |
| C7—N1—V1 | 127.94 (16) | C13—C12—C15 | 121.7 (2) |
| N2—N1—V1 | 116.11 (13) | C14—C13—C12 | 121.3 (2) |
| C8—N2—N1 | 107.35 (18) | C14—C13—H13 | 119.3 |
| C2—O1—V1 | 135.60 (15) | C12—C13—H13 | 119.3 |
| C3—O2—C16 | 117.1 (2) | C13—C14—C9 | 120.3 (2) |
| C8—O3—V1 | 118.96 (14) | C13—C14—H14 | 119.8 |
| C18—O4—V1 | 132.35 (17) | C9—C14—H14 | 119.8 |
| C2—C1—C6 | 120.2 (2) | C12—C15—H15A | 109.5 |
| C2—C1—C7 | 121.1 (2) | C12—C15—H15B | 109.5 |
| C6—C1—C7 | 118.7 (2) | H15A—C15—H15B | 109.5 |
| O1—C2—C1 | 121.2 (2) | C12—C15—H15C | 109.5 |
| O1—C2—C3 | 119.4 (2) | H15A—C15—H15C | 109.5 |
| C1—C2—C3 | 119.4 (2) | H15B—C15—H15C | 109.5 |
| O2—C3—C4 | 125.5 (2) | O2—C16—C17 | 108.1 (2) |
| O2—C3—C2 | 115.9 (2) | O2—C16—H16A | 110.1 |
| C4—C3—C2 | 118.6 (2) | C17—C16—H16A | 110.1 |
| C5—C4—C3 | 121.6 (2) | O2—C16—H16B | 110.1 |
| C5—C4—H4 | 119.2 | C17—C16—H16B | 110.1 |
| C3—C4—H4 | 119.2 | H16A—C16—H16B | 108.4 |
| C6—C5—C4 | 120.7 (2) | C16—C17—H17A | 109.5 |
| C6—C5—H5 | 119.6 | C16—C17—H17B | 109.5 |
| C4—C5—H5 | 119.6 | H17A—C17—H17B | 109.5 |
| C5—C6—C1 | 119.5 (2) | C16—C17—H17C | 109.5 |
| C5—C6—H6 | 120.3 | H17A—C17—H17C | 109.5 |
| C1—C6—H6 | 120.3 | H17B—C17—H17C | 109.5 |
| N1—C7—C1 | 124.2 (2) | O4—C18—H18A | 109.5 |
| N1—C7—H7 | 117.9 | O4—C18—H18B | 109.5 |
| C1—C7—H7 | 117.9 | H18A—C18—H18B | 109.5 |
| N2—C8—O3 | 121.5 (2) | O4—C18—H18C | 109.5 |
| N2—C8—C9 | 120.5 (2) | H18A—C18—H18C | 109.5 |

| | | | |
|---|---|---|---|
| O3—C8—C9 | 118.0 (2) | H18B—C18—H18C | 109.5 |

**Fig. 1**