

# Dioxido[1-[(phenyl)(2-pyridyl)methylene]-4-(*p*-tolyl)thiosemicarbazonato]-vanadium(V) dimethyl sulfoxide solvate

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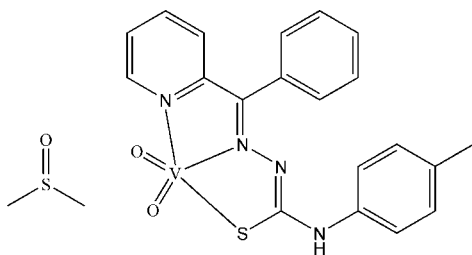
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.059;  $wR$  factor = 0.165; data-to-parameter ratio = 15.3.

In the title compound,  $[\text{V}(\text{C}_{20}\text{H}_{17}\text{N}_4\text{S})\text{O}_2] \cdot \text{C}_2\text{H}_6\text{OS}$ , the organic ligand coordinates the metal atom in a tridentate manner *via* its azomethine nitrogen, thiolate sulfur and pyridyl (py) nitrogen atoms, resulting in two five-membered chelate rings. To match the steric requirements of coordination through the  $\text{N}_{\text{py}}-\text{N}-\text{S}$  chelating system, the 1-[(2-pyridyl)-(phenyl)methylene]-4-(*p*-tolyl)thiosemicarbazonato ligand adopts a configuration different to that of the parent thiosemicarbazone. The V atom shows a distorted trigonal-bipyramidal coordination geometry.

## Related literature

For related literature, see: Ahmad *et al.* (2006); Baran (2000); Beraldo & Gambino (2004); Mendes *et al.* (2006); Philip *et al.* (2005); Sreekanth *et al.* (2003).



## Experimental

### Crystal data

$[\text{V}(\text{C}_{20}\text{H}_{17}\text{N}_4\text{S})\text{O}_2] \cdot \text{C}_2\text{H}_6\text{OS}$   
 $M_r = 506.5$   
Orthorhombic,  $Pbca$   
 $a = 13.9269$  (13) Å  
 $b = 15.399$  (2) Å  
 $c = 22.133$  (4) Å

$V = 4746.4$  (12) Å<sup>3</sup>  
 $Z = 8$   
Mo  $K\alpha$  radiation  
 $\mu = 0.63$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 $0.2 \times 0.2 \times 0.2$  mm

### Data collection

Siemens P4 diffractometer  
Absorption correction: none  
6630 measured reflections  
4420 independent reflections  
2706 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$   
3 standard reflections  
every 247 reflections  
intensity decay: 4%

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$   
 $wR(F^2) = 0.165$   
 $S = 1.02$   
4420 reflections

289 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.85$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.59$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

S1—C8	1.738 (4)	V—N1	2.099 (4)
S1—V	2.3699 (14)	V—N2	2.172 (3)
V—O2	1.599 (4)	N3—C8	1.322 (5)
V—O1	1.606 (4)		
O2—V—O1	111.1 (3)	N1—V—S1	151.15 (10)
O2—V—N2	121.7 (2)	C8—N3—N2	112.1 (3)
O1—V—N2	127.1 (2)	N3—C8—S1	125.0 (3)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{N4}-\text{H4B} \cdots \text{O1A}^i$	0.86	1.96	2.814 (4)	170

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

Data collection: *XSCANS* (Siemens, 1991); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); 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: GK2096).

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**supplementary materials**

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## Dioxido{1-[(phenyl)(2-pyridyl)methylene]-4-(*p*-tolyl)thiosemicarbazonato}vanadium(V) dimethyl sulfoxide solvate

I. C. Mendes, N. L. Speziali and H. Beraldo

### Comment

Thiosemicarbazones and their metal complexes are an important class of compounds with a wide range of pharmacological applications (Beraldo & Gambino, 2004). Vanadium complexes were found to present antimicrobial, antitumor and insulin-enhancing effects (Baran, 2000; Ahmad *et al.*, 2006). Here we report the crystal structure of dioxovanadium(V) complex with 2-benzoylpyridine *N*(4)-(*p*-tolyl)thiosemicarbazone, [VO<sub>2</sub>(2Bz4pT)]·DMSO. 2-Benzoylpyridine *N*(4)-(*p*-tolyl)thiosemicarbazone (H2Bz4pT), crystallizes as the ZE isomer, where Z and E refer to the configuration around C7=N2 and C8—N3 bonds, respectively (Mendes *et al.*, 2006). In the title complex, to match the steric requirements of coordination through the N<sub>py</sub>—N—S chelating system, the deprotonated ligand adopts the EZ configuration (Fig. 1). The C8—N3 bond length changes from 1.361 (3) Å in the free base to 1.322 (5) Å in the complex due to deprotonation of N3 and formation of a new predominantly double bond. In turn, the C8—S1 bond changes from 1.653 (3) Å in H2Bz4pT to 1.738 (4) Å in the complex, in agreement with deprotonation at N3 and formation of a thiolate bond. Deprotonation of the ligand and subsequent coordination to the metal center influences also bond angles. Hence, the N2—N3—C8 bond angle changes from 120.5 (2)° in the free base to 112.1 (3)° in the complex, and N3—C8—S angle changes from 117.9 (2)° in the ligand to 125.0 (3)° in the complex. The atomic arrangement around the vanadium ion has a distorted trigonal bipyramidal geometry (Fig. 2): the interatomic angles in the equatorial plane are in the 111.1 (3)–127.1 (2)° range and the axial angle N1—V—S1 is 151.2 (1)°. The V=O bond distances of 1.606 (4)Å and 1.599 (4)Å are shorter than in the other 2-pyridine thiosemicarbazones vanadium complexes recently published (1.623–1.608 Å; Philip *et al.*, 2005; Sreekanth *et al.*, 2003). A single hydrogen bond was observed between N4—H4B and the oxygen atom from the DMSO molecule. The antifungal activities of the free base and the vanadium complex were evaluated against *Candida albicans*. The thiosemicarbazone proved to be better as antifungal agent than its vanadium complex, probably due to the bulkiness of the complex which does not facilitate its binding to the cell membrane.

### Experimental

Synthesis of 2-benzoylpyridine *N*(4)-(*p*-tolyl) thiosemicarbazone has been reported recently (Mendes *et al.*, 2006). The dioxovanadium(V) complex was obtained by mixing equimolar amounts (3 mmol) of the thiosemicarbazone with [VO(acac)<sub>2</sub>] (acac= acetylacetonate) in ethanol under reflux and stirring for 24 h. The obtained solid was washed with ethanol and ethyl ether and dried in vacuum. Yield 73%. Single crystals of the complex were growth from 1:9 DMSO/acetone solution.

### Refinement

All H atoms were located in a difference map. Nevertheless, their positions were calculated and refined using a riding model approximation, with distance restraints N—H = 0.86 Å, C—H = 0.93–0.96 Å,  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for the methyl groups and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N}, \text{C})$  for the remaining H atoms.

## Figures

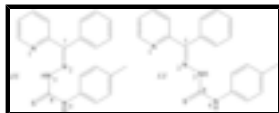


Fig. 1. The ZE and EZ configurational isomers of H2Bz4pT.

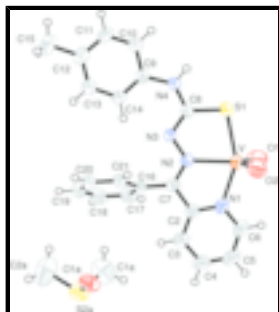


Fig. 2. Molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

## Dioxido[1-[(phenyl)(2-pyridyl)methylene]-4-(p-tolyl)thiosemicarbonato}vanadium(V) dimethyl sulfoxide solvate

### Crystal data

$[\text{V}(\text{C}_{20}\text{H}_{17}\text{N}_4\text{S})\text{O}_2] \cdot \text{C}_2\text{H}_6\text{OS}$

$M_r = 506.5$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 13.9269 (13) \text{ \AA}$

$b = 15.399 (2) \text{ \AA}$

$c = 22.133 (4) \text{ \AA}$

$V = 4746.4 (12) \text{ \AA}^3$

$Z = 8$

$F_{000} = 2096$

$D_x = 1.418 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 33 reflections

$\theta = 6.4\text{--}11.4^\circ$

$\mu = 0.63 \text{ mm}^{-1}$

$T = 298 (2) \text{ K}$

Prismatic, orange

$0.2 \times 0.2 \times 0.2 \text{ mm}$

### Data collection

Siemens P4  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298(2) \text{ K}$

$\omega/2\theta$  scans

Absorption correction: none

6630 measured reflections

4420 independent reflections

2706 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\text{max}} = 25.5^\circ$

$\theta_{\text{min}} = 2.2^\circ$

$h = -13 \rightarrow 16$

$k = -14 \rightarrow 18$

$l = -21 \rightarrow 26$

3 standard reflections

every 247 reflections

intensity decay: 4%

### Refinement

Refinement on  $F^2$

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.059$$

$$wR(F^2) = 0.165$$

$$S = 1.02$$

4420 reflections

289 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 7.659P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.85 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.59 \text{ e } \text{\AA}^{-3}$$

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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.34368 (9)	0.09146 (9)	0.65651 (5)	0.0561 (4)
V	0.50439 (6)	0.13499 (6)	0.67446 (3)	0.0491 (3)
O1	0.4814 (3)	0.2109 (3)	0.72207 (18)	0.0966 (16)
O2	0.5450 (3)	0.0505 (3)	0.70781 (19)	0.0936 (14)
N1	0.6366 (3)	0.1836 (2)	0.64408 (16)	0.0479 (9)
C2	0.6489 (3)	0.1988 (3)	0.58420 (19)	0.0435 (10)
C3	0.7355 (3)	0.2282 (3)	0.5620 (2)	0.0529 (12)
H3	0.7429	0.2395	0.5210	0.064*
C4	0.8112 (4)	0.2408 (4)	0.6015 (2)	0.0629 (14)
H4	0.8704	0.2596	0.5871	0.075*
C5	0.7987 (4)	0.2256 (4)	0.6614 (3)	0.0682 (15)
H5	0.8492	0.2336	0.6883	0.082*
C6	0.7108 (4)	0.1982 (4)	0.6816 (2)	0.0640 (15)
H6	0.7021	0.1895	0.7228	0.077*
C7	0.5650 (3)	0.1763 (3)	0.54705 (18)	0.0364 (9)
N2	0.4935 (2)	0.1421 (2)	0.57668 (14)	0.0362 (8)
N3	0.4155 (2)	0.1158 (2)	0.54342 (14)	0.0374 (8)
C8	0.3450 (3)	0.0871 (3)	0.57804 (17)	0.0364 (9)
N4	0.2660 (2)	0.0531 (2)	0.55245 (14)	0.0400 (8)
H4B	0.2220	0.0376	0.5776	0.048*
C9	0.2431 (3)	0.0384 (3)	0.49082 (18)	0.0374 (9)
C10	0.1491 (3)	0.0141 (3)	0.4783 (2)	0.0459 (11)

## supplementary materials

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H10	0.1056	0.0074	0.5099	0.055*
C11	0.1198 (3)	0.0000 (3)	0.4202 (2)	0.0528 (12)
H11	0.0566	-0.0168	0.4131	0.063*
C12	0.1814 (4)	0.0100 (3)	0.3717 (2)	0.0546 (13)
C13	0.2758 (3)	0.0301 (3)	0.3852 (2)	0.0564 (13)
H13	0.3198	0.0341	0.3537	0.068*
C14	0.3074 (3)	0.0445 (3)	0.44336 (19)	0.0475 (11)
H14	0.3714	0.0581	0.4506	0.057*
C15	0.1458 (4)	-0.0011 (5)	0.3077 (2)	0.0866 (19)
H15A	0.0786	-0.0149	0.3082	0.130*
H15B	0.1805	-0.0472	0.2884	0.130*
H15C	0.1556	0.0519	0.2857	0.130*
C16	0.5663 (3)	0.1908 (3)	0.48091 (18)	0.0361 (9)
C17	0.5761 (3)	0.2748 (3)	0.4579 (2)	0.0539 (12)
H17	0.5829	0.3213	0.4844	0.065*
C18	0.5759 (3)	0.2896 (4)	0.3967 (2)	0.0612 (14)
H18	0.5829	0.3458	0.3819	0.073*
C19	0.5654 (3)	0.2216 (4)	0.3572 (2)	0.0605 (14)
H19	0.5647	0.2317	0.3158	0.073*
C20	0.5559 (3)	0.1383 (3)	0.3789 (2)	0.0527 (12)
H20	0.5492	0.0923	0.3520	0.063*
C21	0.5564 (3)	0.1225 (3)	0.44055 (18)	0.0414 (10)
H21	0.5501	0.0660	0.4549	0.050*
S2A	0.90467 (10)	0.09940 (10)	0.35510 (7)	0.0709 (4)
O1A	0.8871 (2)	0.0091 (2)	0.37672 (15)	0.0626 (9)
C1A	0.8368 (5)	0.1666 (4)	0.4021 (3)	0.102 (2)
H1AA	0.8661	0.1692	0.4414	0.152*
H1AB	0.7729	0.1437	0.4058	0.152*
H1AC	0.8340	0.2239	0.3851	0.152*
C2A	0.8358 (7)	0.1097 (5)	0.2909 (3)	0.127 (3)
H2AA	0.8627	0.0747	0.2593	0.191*
H2AB	0.8349	0.1694	0.2784	0.191*
H2AC	0.7715	0.0908	0.2992	0.191*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0483 (7)	0.0871 (10)	0.0330 (6)	-0.0164 (7)	0.0038 (5)	0.0001 (6)
V	0.0433 (4)	0.0734 (6)	0.0307 (4)	-0.0005 (4)	-0.0021 (3)	-0.0039 (4)
O1	0.064 (3)	0.147 (4)	0.079 (3)	-0.018 (3)	0.008 (2)	-0.067 (3)
O2	0.058 (2)	0.139 (4)	0.084 (3)	0.005 (3)	0.002 (2)	0.055 (3)
N1	0.046 (2)	0.059 (2)	0.038 (2)	-0.0004 (19)	-0.0084 (17)	-0.0110 (18)
C2	0.042 (3)	0.045 (3)	0.043 (2)	-0.002 (2)	-0.005 (2)	-0.009 (2)
C3	0.042 (3)	0.063 (3)	0.054 (3)	-0.009 (2)	-0.002 (2)	-0.006 (2)
C4	0.043 (3)	0.073 (4)	0.073 (4)	-0.012 (3)	-0.006 (3)	-0.010 (3)
C5	0.048 (3)	0.087 (4)	0.070 (4)	-0.007 (3)	-0.016 (3)	-0.021 (3)
C6	0.061 (3)	0.088 (4)	0.044 (3)	-0.003 (3)	-0.012 (2)	-0.015 (3)
C7	0.036 (2)	0.032 (2)	0.041 (2)	-0.0014 (18)	-0.0018 (19)	-0.0046 (18)

N2	0.0353 (18)	0.0397 (19)	0.0336 (17)	-0.0065 (16)	-0.0016 (15)	-0.0045 (15)
N3	0.0336 (19)	0.049 (2)	0.0294 (17)	-0.0089 (16)	-0.0014 (15)	-0.0025 (15)
C8	0.040 (2)	0.037 (2)	0.032 (2)	-0.0009 (19)	0.0031 (19)	0.0002 (18)
N4	0.0331 (19)	0.053 (2)	0.0337 (18)	-0.0111 (17)	0.0018 (15)	0.0016 (16)
C9	0.040 (2)	0.033 (2)	0.039 (2)	-0.0012 (19)	-0.0027 (19)	-0.0002 (18)
C10	0.036 (2)	0.054 (3)	0.047 (2)	-0.007 (2)	0.001 (2)	0.000 (2)
C11	0.041 (3)	0.067 (3)	0.051 (3)	-0.006 (2)	-0.014 (2)	-0.009 (2)
C12	0.061 (3)	0.061 (3)	0.042 (3)	0.000 (3)	-0.012 (2)	-0.005 (2)
C13	0.050 (3)	0.078 (4)	0.041 (3)	-0.007 (3)	0.004 (2)	-0.008 (2)
C14	0.035 (2)	0.065 (3)	0.043 (2)	-0.008 (2)	-0.001 (2)	-0.006 (2)
C15	0.082 (4)	0.130 (5)	0.048 (3)	-0.010 (4)	-0.015 (3)	-0.016 (3)
C16	0.028 (2)	0.039 (2)	0.041 (2)	-0.0061 (18)	-0.0005 (17)	0.0006 (19)
C17	0.053 (3)	0.045 (3)	0.063 (3)	-0.011 (2)	0.000 (2)	0.003 (2)
C18	0.052 (3)	0.060 (3)	0.072 (4)	-0.007 (3)	-0.002 (3)	0.028 (3)
C19	0.048 (3)	0.092 (4)	0.041 (3)	-0.006 (3)	0.000 (2)	0.020 (3)
C20	0.049 (3)	0.070 (3)	0.039 (2)	-0.005 (3)	0.001 (2)	-0.007 (2)
C21	0.040 (2)	0.045 (3)	0.040 (2)	-0.005 (2)	0.0011 (19)	0.001 (2)
S2A	0.0606 (9)	0.0785 (10)	0.0736 (9)	-0.0067 (8)	0.0075 (7)	0.0188 (8)
O1A	0.054 (2)	0.062 (2)	0.072 (2)	-0.0053 (17)	0.0155 (17)	0.0183 (18)
C1A	0.125 (6)	0.063 (4)	0.116 (6)	-0.003 (4)	0.021 (5)	-0.018 (4)
C2A	0.175 (9)	0.114 (6)	0.093 (5)	-0.011 (6)	-0.041 (6)	0.014 (5)

*Geometric parameters (Å, °)*

S1—C8	1.738 (4)	C11—H11	0.9300
S1—V	2.3699 (14)	C12—C13	1.383 (7)
V—O2	1.599 (4)	C12—C15	1.512 (6)
V—O1	1.606 (4)	C13—C14	1.379 (6)
V—N1	2.099 (4)	C13—H13	0.9300
V—N2	2.172 (3)	C14—H14	0.9300
N1—C6	1.344 (6)	C15—H15A	0.9600
N1—C2	1.357 (5)	C15—H15B	0.9600
C2—C3	1.379 (6)	C15—H15C	0.9600
C2—C7	1.469 (6)	C16—C21	1.387 (6)
C3—C4	1.384 (6)	C16—C17	1.397 (6)
C3—H3	0.9300	C17—C18	1.375 (7)
C4—C5	1.357 (7)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.372 (7)
C5—C6	1.370 (7)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.375 (7)
C6—H6	0.9300	C19—H19	0.9300
C7—N2	1.304 (5)	C20—C21	1.386 (6)
C7—C16	1.481 (6)	C20—H20	0.9300
N2—N3	1.374 (4)	C21—H21	0.9300
N3—C8	1.322 (5)	S2A—O1A	1.491 (4)
C8—N4	1.344 (5)	S2A—C2A	1.722 (7)
N4—C9	1.418 (5)	S2A—C1A	1.746 (6)
N4—H4B	0.8600	C1A—H1AA	0.9600
C9—C14	1.383 (6)	C1A—H1AB	0.9600

## supplementary materials

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C9—C10	1.390 (6)	C1A—H1AC	0.9600
C10—C11	1.367 (6)	C2A—H2AA	0.9600
C10—H10	0.9300	C2A—H2AB	0.9600
C11—C12	1.384 (7)	C2A—H2AC	0.9600
C8—S1—V	99.71 (15)	C12—C11—H11	119.1
O2—V—O1	111.1 (3)	C13—C12—C11	116.6 (4)
O2—V—N1	97.32 (18)	C13—C12—C15	122.7 (5)
O1—V—N1	97.21 (18)	C11—C12—C15	120.8 (5)
O2—V—N2	121.7 (2)	C14—C13—C12	122.7 (4)
O1—V—N2	127.1 (2)	C14—C13—H13	118.6
N1—V—N2	73.97 (13)	C12—C13—H13	118.6
O2—V—S1	100.46 (16)	C13—C14—C9	119.5 (4)
O1—V—S1	97.33 (14)	C13—C14—H14	120.3
N1—V—S1	151.15 (10)	C9—C14—H14	120.3
N2—V—S1	77.38 (9)	C12—C15—H15A	109.5
C6—N1—C2	118.5 (4)	C12—C15—H15B	109.5
C6—N1—V	122.4 (3)	H15A—C15—H15B	109.5
C2—N1—V	119.0 (3)	C12—C15—H15C	109.5
N1—C2—C3	121.0 (4)	H15A—C15—H15C	109.5
N1—C2—C7	114.0 (4)	H15B—C15—H15C	109.5
C3—C2—C7	125.0 (4)	C21—C16—C17	118.5 (4)
C2—C3—C4	119.2 (5)	C21—C16—C7	121.4 (4)
C2—C3—H3	120.4	C17—C16—C7	120.1 (4)
C4—C3—H3	120.4	C18—C17—C16	120.8 (5)
C5—C4—C3	119.6 (5)	C18—C17—H17	119.6
C5—C4—H4	120.2	C16—C17—H17	119.6
C3—C4—H4	120.2	C19—C18—C17	120.1 (5)
C4—C5—C6	119.1 (5)	C19—C18—H18	120.0
C4—C5—H5	120.4	C17—C18—H18	120.0
C6—C5—H5	120.4	C18—C19—C20	120.0 (4)
N1—C6—C5	122.5 (5)	C18—C19—H19	120.0
N1—C6—H6	118.8	C20—C19—H19	120.0
C5—C6—H6	118.8	C19—C20—C21	120.5 (5)
N2—C7—C2	114.9 (4)	C19—C20—H20	119.8
N2—C7—C16	124.5 (3)	C21—C20—H20	119.8
C2—C7—C16	120.6 (4)	C20—C21—C16	120.0 (4)
C7—N2—N3	117.0 (3)	C20—C21—H21	120.0
C7—N2—V	117.9 (3)	C16—C21—H21	120.0
N3—N2—V	125.0 (2)	O1A—S2A—C2A	105.0 (3)
C8—N3—N2	112.1 (3)	O1A—S2A—C1A	105.8 (3)
N3—C8—N4	119.6 (3)	C2A—S2A—C1A	97.8 (4)
N3—C8—S1	125.0 (3)	S2A—C1A—H1AA	109.5
N4—C8—S1	115.3 (3)	S2A—C1A—H1AB	109.5
C8—N4—C9	130.6 (3)	H1AA—C1A—H1AB	109.5
C8—N4—H4B	114.7	S2A—C1A—H1AC	109.5
C9—N4—H4B	114.7	H1AA—C1A—H1AC	109.5
C14—C9—C10	118.5 (4)	H1AB—C1A—H1AC	109.5
C14—C9—N4	125.1 (4)	S2A—C2A—H2AA	109.5
C10—C9—N4	116.4 (4)	S2A—C2A—H2AB	109.5



C11—C10—C9	120.7 (4)	H2AA—C2A—H2AB	109.5
C11—C10—H10	119.6	S2A—C2A—H2AC	109.5
C9—C10—H10	119.6	H2AA—C2A—H2AC	109.5
C10—C11—C12	121.8 (4)	H2AB—C2A—H2AC	109.5
C10—C11—H11	119.1		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N4—H4B $\cdots$ O1A <sup>i</sup>	0.86	1.96	2.814 (4)	170

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

Fig. 1

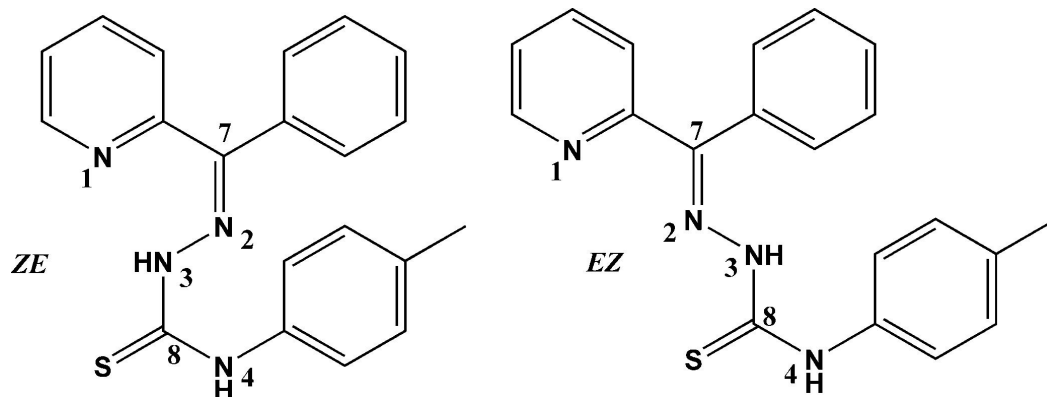


Fig. 2

