

# 3,6,14,17-Tetramethoxy-22,23-diphenyl-1,10,12,21-tetraazahexacyclo-[19.2.1.0<sup>2,7</sup>.0<sup>10,23</sup>.0<sup>12,22</sup>.0<sup>13,18</sup>]tetracos-2(7),3,5,13(18),14,16-hexaene-11,24-dithione

Yan Yang

Key Laboratory of Pesticides and Chemical Biology of Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

Correspondence e-mail: yanyang20100203@gmail.com

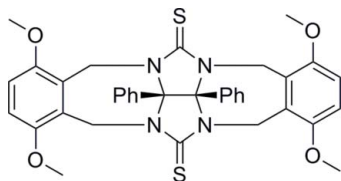
Received 26 April 2010; accepted 9 June 2010

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.056;  $wR$  factor = 0.162; data-to-parameter ratio = 16.9.

The title compound,  $\text{C}_{36}\text{H}_{34}\text{N}_4\text{O}_4\text{S}_2$ , is a thioglycoluril derivative, which bears two phenyl substituents on its convex face and two methoxy substituted *o*-xylylenes as sidewalls of the molecular clip. There is one half-molecule in the asymmetric unit: a crystallographic twofold axis generates the complete molecule. The non-planar seven-membered rings adopt chair conformations, while the two five-membered rings exhibit envelope conformations and make a dihedral angle of  $68.46$  ( $12$ )°. The O atoms of the methoxy groups are coplanar with the six-membered *o*-xylylene sidewalls.

## Related literature

For related structures, see: Broan *et al.* (1989); Cao *et al.* (2009); Wang *et al.* (2006); Wang & Xi (2009); Wu & Sun, (2009). For further synthetic details, see: Broan *et al.* (1989); Wu *et al.* (2002). The rigid concave shape of glycoluril makes it a versatile building block in supramolecular chemistry, see: Gao *et al.* (2009); Rowan *et al.* (1999); Hof *et al.* (2002); Kolbel & Menger (2001); Wu *et al.* (2002); Kang *et al.* (2004).



## Experimental

### Crystal data

$\text{C}_{36}\text{H}_{34}\text{N}_4\text{O}_4\text{S}_2$	$V = 3257.3$ (5) Å <sup>3</sup>
$M_r = 650.79$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 17.9993$ (15) Å	$\mu = 0.21$ mm <sup>-1</sup>
$b = 12.5069$ (11) Å	$T = 298$ K
$c = 16.0934$ (12) Å	$0.23 \times 0.20 \times 0.10$ mm
$\beta = 115.961$ (3)°	

### Data collection

Bruker SMART CCD area-detector diffractometer	3546 independent reflections
13570 measured reflections	2279 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.067$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$	210 parameters
$wR(F^2) = 0.162$	H-atom parameters constrained
$S = 0.98$	$\Delta\rho_{\text{max}} = 0.29$ e Å <sup>-3</sup>
3546 reflections	$\Delta\rho_{\text{min}} = -0.24$ e Å <sup>-3</sup>

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

The author thanks Professor An-Xin Wu for technical assistance and Dr Meng Xiang-Gao for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2304).

## References

- Broan, C. J., Butler, A. R., Reed, D. & Sadler, I. H. (1989). *J. Chem. Soc. Perkin Trans. 2*, pp. 731–740.
- Bruker (2001). *SMART* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cao, L., Ding, J., Yin, G., Gao, M., Li, Y. & Wu, A. (2009). *Synlett*, pp. 1445–1448.
- Gao, M., Cao, L., Wang, Z., Sun, J., She, N. & Wu, A. (2009). *Synlett*, pp. 315–319.
- Hof, F., Craig, S. L., Nuckolls, C. & Rebek, J. Jr (2002). *Angew. Chem. Int. Ed.* **41**, 1488–1508.
- Kang, J., Jo, J.-H. & In, S. (2004). *Tetrahedron Lett.* **45**, 5225–5228.
- Kolbel, M. & Menger, F. M. (2001). *Chem. Commun.* pp. 275–276.
- Rowan, A. E., Elemans, J. A. A. W. & Nolte, R. J. M. (1999). *Acc. Chem. Res.* **32**, 995–1006.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Wang, Z. & Xi, H. (2009). *Acta Cryst.* **E65**, o1426.
- Wang, Z., Zhou, B., Chen, Y., Yin, G., Li, Y., Wu, A. & Isaacs, L. (2006). *J. Org. Chem.* **71**, 4502–4508.
- Wu, A., Chakraborty, A., Witt, D., Lagona, J., Damkaci, F., Ofori, M. A., Chiles, J. K., Fettinger, J. C. & Isaacs, L. (2002). *J. Org. Chem.* **67**, 5817–5830.
- Wu, Y. & Sun, Y. (2009). *Acta Cryst.* **E65**, o1715.

**supplementary materials**

*Acta Cryst.* (2010). E66, o1673 [ doi:10.1107/S160053681002204X ]

**3,6,14,17-Tetramethoxy-22,23-diphenyl-1,10,12,21-tetraazahexacyclo[19.2.1.0<sup>2,7</sup>.0<sup>10,23</sup>.0<sup>12,22</sup>.0<sup>13,18</sup>]tetracos-2(7),3,5,13(18),14,16-hexaene-11,24-dithione**

**Y. Yang**

**Comment**

The rigid concave shape of glycoluril makes it a versatile building block to construct various supramolecular objects (Gao *et al.*, 2009), including molecular clips and molecular baskets (Rowan *et al.*, 1999), molecular capsules (Hof *et al.*, 2002), xerogels (Kolbel & Menger, 2001), the cucurbit[n]uril family (Wu *et al.*, 2002), and anion-binding receptors (Kang *et al.*, 2004). Based on the previous studies (Broan *et al.*, 1989; Cao *et al.*, 2009; Wang *et al.*, 2006; Wang & Xi, 2009; Wu & Sun, 2009), we report here the structure of the title thioglycoluril derivative (Fig. 1), which is a potential receptor in supramolecular chemistry.

There is one half-molecule in the asymmetric unit. The non-planar seven-membered rings adopt chair conformations, while the two five-membered rings have envelope conformation and the dihedral angle between them is 68.46°. The methoxy groups on sidewalls are coplanar with the six-membered o-xylene sidewalls. The molecule contains three nonclassical intramolecular C—H⋯S, C—H⋯O and C—H⋯N hydrogen bonds, and its crystal structure is stabilized mostly by intermolecular C—H⋯π interactions (Table 1).

**Experimental**

The thioglycoluril was synthesized according to a literature procedure, see : Broan *et al.*, (1989). Preparation of the title compound: A solution of thioglycoluril (326 mg, 1.00 mmol), paraformaldehyde (120 mg, 4.00 mmol) and 1,4-dimethoxybenzene (304 mg, 2.20 mmol) in TFA (5 ml) was stirred and heated at reflux for 6 h. After rotary evaporation the residue was chromatographed to yield the title compound (521 mg, 0.80 mmol, 80%). Crystals of (I) suitable for X-ray diffraction were grown by slow evaporation of a dichloromethane-methanol (1:2) solution of the title compound under 293 K.

**Refinement**

All H atoms were positioned in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å and U<sub>iso</sub>(H) = 1.2U<sub>eq</sub>(C) or U<sub>iso</sub>(H) = 1.5U<sub>eq</sub>(C).

## Figures

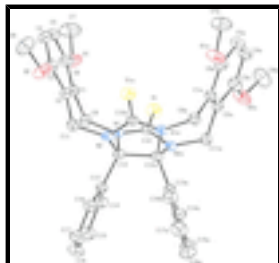


Fig. 1. A view of (I), showing the atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability level.

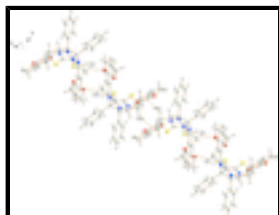


Fig. 2. Packing of (I) with C—H... $\pi$  interactions drawn as dashed lines showing the formation of a one-dimensional chain.

**3,6,14,17-Tetramethoxy-22,23-diphenyl-1,10,12,21-tetraazahexacyclo[19.2.1.0<sup>2,7</sup>.0<sup>10,23</sup>.0<sup>12,22</sup>.0<sup>13,18</sup>]tetracosane-2(7),3,5,13 (18),14,16-hexaene-11,24-dithione**

### Crystal data

$C_{36}H_{34}N_4O_4S_2$

$M_r = 650.79$

Monoclinic,  $C2/c$

Hall symbol:  $-C\ 2yc$

$a = 17.9993$  (15) Å

$b = 12.5069$  (11) Å

$c = 16.0934$  (12) Å

$\beta = 115.961$  (3)°

$V = 3257.3$  (5) Å<sup>3</sup>

$Z = 4$

$F(000) = 1368$

$D_x = 1.327$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2697 reflections

$\theta = 2.5$ – $21.3$ °

$\mu = 0.21$  mm<sup>-1</sup>

$T = 298$  K

Block, colorless

$0.23 \times 0.20 \times 0.10$  mm

### Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

phi and  $\omega$  scans

13570 measured reflections

3546 independent reflections

2279 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.067$

$\theta_{max} = 27.0$ °,  $\theta_{min} = 2.1$ °

$h = -22 \rightarrow 13$

$k = -15 \rightarrow 15$

$l = -19 \rightarrow 20$

### Refinement

Refinement on  $F^2$

Primary atom site location: structure-invariant direct methods

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.056$$

$$wR(F^2) = 0.162$$

$$S = 0.98$$

3546 reflections

210 parameters

0 restraints

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0878P)^2]$$

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

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

$$\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$$

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.11451 (4)	0.22118 (5)	0.14339 (5)	0.0528 (3)
N1	0.09215 (11)	0.31734 (13)	0.27979 (13)	0.0335 (5)
N2	-0.00738 (11)	0.34780 (13)	0.14082 (13)	0.0325 (4)
C13	0.07957 (13)	0.50126 (16)	0.32973 (15)	0.0343 (5)
C9	0.16813 (14)	0.27755 (17)	0.35521 (17)	0.0388 (6)
H9A	0.1970	0.3371	0.3949	0.047*
H9B	0.2036	0.2489	0.3294	0.047*
C12	0.03855 (13)	0.39284 (16)	0.29759 (15)	0.0306 (5)
C10	0.06573 (14)	0.29489 (16)	0.18917 (16)	0.0326 (5)
O2	0.06197 (14)	0.16264 (16)	0.57355 (15)	0.0713 (6)
O1	0.24132 (13)	0.08009 (14)	0.37734 (15)	0.0683 (6)
C1	0.15415 (14)	0.19204 (17)	0.41322 (17)	0.0393 (6)
C2	0.10798 (15)	0.21274 (17)	0.46227 (17)	0.0406 (6)
C6	0.19350 (16)	0.09225 (18)	0.42349 (19)	0.0477 (7)
C18	0.13789 (15)	0.53676 (19)	0.30210 (19)	0.0497 (7)
H18	0.1560	0.4916	0.2688	0.060*
C11	-0.06462 (15)	0.31850 (18)	0.04628 (16)	0.0392 (6)
H11A	-0.0343	0.3157	0.0092	0.047*
H11B	-0.1060	0.3742	0.0209	0.047*
C3	0.10368 (17)	0.1344 (2)	0.52320 (19)	0.0512 (7)
C14	0.05429 (16)	0.56979 (18)	0.37978 (18)	0.0463 (7)
H14	0.0150	0.5469	0.3988	0.056*
C4	0.14195 (17)	0.0364 (2)	0.5309 (2)	0.0578 (8)

## supplementary materials

---

H4	0.1379	-0.0156	0.5701	0.069*
C17	0.16966 (18)	0.6394 (2)	0.3237 (2)	0.0655 (9)
H17	0.2086	0.6631	0.3045	0.079*
C5	0.18588 (18)	0.0156 (2)	0.4811 (2)	0.0564 (8)
H5	0.2108	-0.0508	0.4863	0.068*
C15	0.0865 (2)	0.6717 (2)	0.4019 (2)	0.0638 (9)
H15	0.0693	0.7170	0.4360	0.077*
C16	0.1438 (2)	0.7055 (2)	0.3733 (2)	0.0731 (10)
H16	0.1654	0.7742	0.3878	0.088*
C7	0.2729 (2)	-0.0224 (2)	0.3750 (3)	0.0859 (11)
H7A	0.2924	-0.0550	0.4348	0.129*
H7B	0.3178	-0.0162	0.3583	0.129*
H7C	0.2301	-0.0658	0.3302	0.129*
C8	0.0599 (2)	0.0907 (3)	0.6401 (2)	0.0865 (11)
H8A	0.0241	0.0319	0.6094	0.130*
H8B	0.0396	0.1269	0.6787	0.130*
H8C	0.1146	0.0643	0.6775	0.130*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0520 (5)	0.0520 (4)	0.0612 (5)	0.0130 (3)	0.0311 (4)	-0.0081 (3)
N1	0.0300 (11)	0.0293 (9)	0.0435 (12)	0.0043 (7)	0.0181 (9)	0.0014 (8)
N2	0.0341 (11)	0.0273 (9)	0.0390 (11)	0.0020 (8)	0.0189 (9)	-0.0016 (8)
C13	0.0316 (13)	0.0300 (11)	0.0397 (13)	-0.0029 (9)	0.0141 (10)	0.0006 (9)
C9	0.0268 (13)	0.0385 (13)	0.0466 (14)	0.0035 (10)	0.0118 (11)	0.0042 (10)
C12	0.0317 (12)	0.0264 (10)	0.0391 (12)	0.0013 (9)	0.0205 (10)	0.0006 (9)
C10	0.0327 (13)	0.0270 (11)	0.0395 (14)	-0.0012 (9)	0.0170 (11)	0.0011 (9)
O2	0.0922 (16)	0.0662 (13)	0.0746 (14)	0.0174 (11)	0.0543 (13)	0.0311 (11)
O1	0.0756 (15)	0.0481 (11)	0.0968 (17)	0.0248 (10)	0.0521 (13)	0.0162 (10)
C1	0.0328 (14)	0.0343 (12)	0.0433 (14)	0.0000 (10)	0.0097 (11)	0.0030 (10)
C2	0.0390 (14)	0.0331 (12)	0.0430 (14)	-0.0015 (10)	0.0118 (12)	0.0037 (10)
C6	0.0452 (16)	0.0364 (13)	0.0582 (17)	0.0053 (11)	0.0197 (13)	0.0014 (11)
C18	0.0428 (16)	0.0428 (14)	0.0692 (19)	-0.0048 (11)	0.0300 (14)	0.0017 (12)
C11	0.0397 (14)	0.0408 (13)	0.0357 (13)	0.0020 (10)	0.0153 (11)	-0.0017 (10)
C3	0.0549 (18)	0.0474 (15)	0.0536 (17)	-0.0009 (13)	0.0259 (14)	0.0083 (12)
C14	0.0582 (17)	0.0334 (13)	0.0518 (16)	-0.0035 (11)	0.0284 (14)	-0.0037 (11)
C4	0.063 (2)	0.0437 (15)	0.0596 (18)	0.0013 (13)	0.0207 (16)	0.0190 (13)
C17	0.0486 (18)	0.0531 (17)	0.091 (2)	-0.0183 (14)	0.0267 (17)	0.0117 (16)
C5	0.065 (2)	0.0345 (14)	0.0639 (19)	0.0073 (12)	0.0226 (16)	0.0073 (13)
C15	0.090 (2)	0.0359 (14)	0.0624 (19)	-0.0065 (15)	0.0304 (17)	-0.0115 (13)
C16	0.084 (3)	0.0387 (16)	0.080 (2)	-0.0232 (16)	0.021 (2)	-0.0042 (15)
C7	0.112 (3)	0.055 (2)	0.113 (3)	0.0199 (19)	0.070 (3)	-0.0035 (18)
C8	0.099 (3)	0.095 (3)	0.076 (2)	0.009 (2)	0.048 (2)	0.036 (2)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

S1—C10	1.652 (2)	C6—C5	1.381 (4)
N1—C10	1.351 (3)	C18—C17	1.386 (4)

N1—C9	1.462 (3)	C18—H18	0.9300
N1—C12	1.465 (3)	C11—C2 <sup>i</sup>	1.511 (3)
N2—C10	1.371 (3)	C11—H11A	0.9700
N2—C12 <sup>i</sup>	1.450 (3)	C11—H11B	0.9700
N2—C11	1.462 (3)	C3—C4	1.384 (4)
C13—C18	1.381 (3)	C14—C15	1.381 (3)
C13—C14	1.382 (3)	C14—H14	0.9300
C13—C12	1.522 (3)	C4—C5	1.375 (4)
C9—C1	1.511 (3)	C4—H4	0.9300
C9—H9A	0.9700	C17—C16	1.364 (4)
C9—H9B	0.9700	C17—H17	0.9300
C12—N2 <sup>i</sup>	1.450 (3)	C5—H5	0.9300
C12—C12 <sup>i</sup>	1.553 (4)	C15—C16	1.369 (4)
O2—C3	1.370 (3)	C15—H15	0.9300
O2—C8	1.412 (3)	C16—H16	0.9300
O1—C6	1.369 (3)	C7—H7A	0.9600
O1—C7	1.410 (3)	C7—H7B	0.9600
C1—C2	1.398 (3)	C7—H7C	0.9600
C1—C6	1.409 (3)	C8—H8A	0.9600
C2—C3	1.412 (3)	C8—H8B	0.9600
C2—C11 <sup>i</sup>	1.511 (3)	C8—H8C	0.9600
C10—N1—C9	125.79 (19)	N2—C11—H11A	108.6
C10—N1—C12	113.23 (17)	C2 <sup>i</sup> —C11—H11A	108.6
C9—N1—C12	120.91 (18)	N2—C11—H11B	108.6
C10—N2—C12 <sup>i</sup>	111.24 (18)	C2 <sup>i</sup> —C11—H11B	108.6
C10—N2—C11	122.26 (18)	H11A—C11—H11B	107.6
C12 <sup>i</sup> —N2—C11	120.09 (18)	O2—C3—C4	123.7 (2)
C18—C13—C14	118.6 (2)	O2—C3—C2	116.3 (2)
C18—C13—C12	120.1 (2)	C4—C3—C2	120.0 (3)
C14—C13—C12	121.1 (2)	C15—C14—C13	121.0 (3)
N1—C9—C1	113.92 (19)	C15—C14—H14	119.5
N1—C9—H9A	108.8	C13—C14—H14	119.5
C1—C9—H9A	108.8	C5—C4—C3	120.4 (2)
N1—C9—H9B	108.8	C5—C4—H4	119.8
C1—C9—H9B	108.8	C3—C4—H4	119.8
H9A—C9—H9B	107.7	C16—C17—C18	120.0 (3)
N2 <sup>i</sup> —C12—N1	111.61 (16)	C16—C17—H17	120.0
N2 <sup>i</sup> —C12—C13	112.90 (18)	C18—C17—H17	120.0
N1—C12—C13	112.20 (18)	C4—C5—C6	120.8 (2)
N2 <sup>i</sup> —C12—C12 <sup>i</sup>	103.2 (2)	C4—C5—H5	119.6
N1—C12—C12 <sup>i</sup>	100.82 (17)	C6—C5—H5	119.6
C13—C12—C12 <sup>i</sup>	115.23 (12)	C16—C15—C14	119.4 (3)
N1—C10—N2	108.02 (18)	C16—C15—H15	120.3
N1—C10—S1	126.35 (17)	C14—C15—H15	120.3
N2—C10—S1	125.57 (17)	C17—C16—C15	120.7 (3)
C3—O2—C8	119.2 (2)	C17—C16—H16	119.7

## supplementary materials

---

C6—O1—C7	118.2 (2)	C15—C16—H16	119.7
C2—C1—C6	119.4 (2)	O1—C7—H7A	109.5
C2—C1—C9	121.2 (2)	O1—C7—H7B	109.5
C6—C1—C9	119.2 (2)	H7A—C7—H7B	109.5
C1—C2—C3	119.4 (2)	O1—C7—H7C	109.5
C1—C2—C11 <sup>i</sup>	121.4 (2)	H7A—C7—H7C	109.5
C3—C2—C11 <sup>i</sup>	119.2 (2)	H7B—C7—H7C	109.5
O1—C6—C5	123.9 (2)	O2—C8—H8A	109.5
O1—C6—C1	116.0 (2)	O2—C8—H8B	109.5
C5—C6—C1	120.0 (3)	H8A—C8—H8B	109.5
C13—C18—C17	120.3 (3)	O2—C8—H8C	109.5
C13—C18—H18	119.8	H8A—C8—H8C	109.5
C17—C18—H18	119.8	H8B—C8—H8C	109.5
N2—C11—C2 <sup>i</sup>	114.50 (19)		
C10—N1—C9—C1	-106.3 (3)	C7—O1—C6—C5	11.7 (4)
C12—N1—C9—C1	77.1 (3)	C7—O1—C6—C1	-171.6 (3)
C10—N1—C12—N2 <sup>i</sup>	122.1 (2)	C2—C1—C6—O1	-176.5 (2)
C9—N1—C12—N2 <sup>i</sup>	-60.9 (2)	C9—C1—C6—O1	-1.2 (3)
C10—N1—C12—C13	-110.1 (2)	C2—C1—C6—C5	0.4 (4)
C9—N1—C12—C13	66.9 (2)	C9—C1—C6—C5	175.7 (2)
C10—N1—C12—C12 <sup>i</sup>	13.1 (2)	C14—C13—C18—C17	-0.5 (4)
C9—N1—C12—C12 <sup>i</sup>	-169.92 (18)	C12—C13—C18—C17	173.8 (2)
C18—C13—C12—N2 <sup>i</sup>	155.7 (2)	C10—N2—C11—C2 <sup>i</sup>	70.0 (3)
C14—C13—C12—N2 <sup>i</sup>	-30.1 (3)	C12 <sup>i</sup> —N2—C11—C2 <sup>i</sup>	-79.4 (2)
C18—C13—C12—N1	28.6 (3)	C8—O2—C3—C4	2.6 (4)
C14—C13—C12—N1	-157.3 (2)	C8—O2—C3—C2	-175.9 (3)
C18—C13—C12—C12 <sup>i</sup>	-86.0 (3)	C1—C2—C3—O2	175.8 (2)
C14—C13—C12—C12 <sup>i</sup>	88.1 (3)	C11 <sup>i</sup> —C2—C3—O2	-2.3 (4)
C9—N1—C10—N2	-179.57 (19)	C1—C2—C3—C4	-2.8 (4)
C12—N1—C10—N2	-2.7 (2)	C11 <sup>i</sup> —C2—C3—C4	179.0 (2)
C9—N1—C10—S1	-2.1 (3)	C18—C13—C14—C15	0.0 (4)
C12—N1—C10—S1	174.75 (16)	C12—C13—C14—C15	-174.3 (2)
C12 <sup>i</sup> —N2—C10—N1	-10.2 (2)	O2—C3—C4—C5	-177.0 (3)
C11—N2—C10—N1	-162.05 (19)	C2—C3—C4—C5	1.5 (4)
C12 <sup>i</sup> —N2—C10—S1	172.29 (15)	C13—C18—C17—C16	0.6 (4)
C11—N2—C10—S1	20.5 (3)	C3—C4—C5—C6	0.8 (4)
N1—C9—C1—C2	-61.3 (3)	O1—C6—C5—C4	174.9 (2)
N1—C9—C1—C6	123.5 (2)	C1—C6—C5—C4	-1.8 (4)
C6—C1—C2—C3	1.8 (4)	C13—C14—C15—C16	0.5 (4)
C9—C1—C2—C3	-173.4 (2)	C18—C17—C16—C15	-0.2 (5)
C6—C1—C2—C11 <sup>i</sup>	180.0 (2)	C14—C15—C16—C17	-0.4 (5)
C9—C1—C2—C11 <sup>i</sup>	4.8 (3)		

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



Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C1–C6 ring.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C9—H9A···Cg1 <sup>ii</sup>	0.97	2.70	3.540	145.
C11—H11A···O2 <sup>ii</sup>	0.97	2.26	2.757 (3)	111
C14—H14···N2 <sup>ii</sup>	0.93	2.56	2.879 (3)	101
C18—H18···N1	0.93	2.51	2.842 (3)	102
C9—H9B···S1	0.97	2.73	3.189 (3)	110
C9—H9B···O1	0.97	2.25	2.748 (3)	111

Symmetry codes: (ii)  $-x, y, -z+1/2$ .

Fig. 1

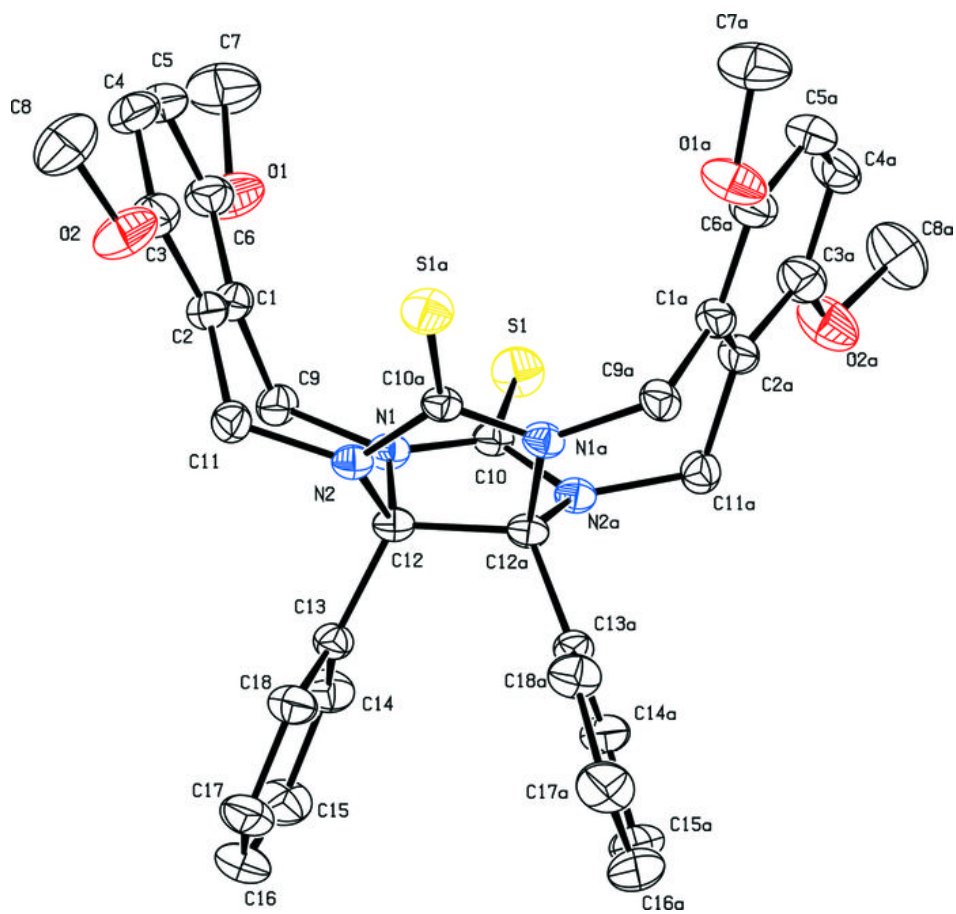


Fig. 2

