$a = 8.939\,(2)$ Å
$b = 9.360\,(2)$ Å
$c = 11.438\,(2)$ Å
$V = 957.0\,(3)$ Å^3
$Z = 4$
$D_x = 1.830$ Mg m^{-3}
D_m not measured

$\theta = 10.0\text{–}11.5°$
$\mu = 0.839$ mm^{-1}
$T = 143\,(2)$ K
Prism
$0.5 \times 0.4 \times 0.4$ mm
Colourless

Data collection

Stoe Stadi-4 diffractometer
ω/θ scans
Absorption correction: none
2418 measured reflections
2195 independent reflections
2162 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.0188$

$\theta_{\rm max} = 27.51°$
$h = -11 \rightarrow 11$
$k = 0 \rightarrow 12$
$l = 0 \rightarrow 14$
3 standard reflections
  frequency: 60 min
  intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0201$
$wR(F^2) = 0.0575$
$S = 1.073$
2188 reflections
130 parameters
H atoms: methyls refined as rigid groups
$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2 + 0.2238P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$

$\Delta\rho_{\rm max} = 0.247$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.220$ e Å^{-3}
Extinction correction: *SHELXL*93
Extinction coefficient: 0.0221 (14)
Scattering factors from *International Tables for Crystallography* (Vol. C)
Absolute structure: Flack (1983)
Flack parameter = 0.02 (5)

Table 1. *Selected geometric parameters (Å, °)*

N1—C3	1.408 (2)	S2—O4	1.4237 (13)
N1—S1	1.7168 (12)	S2—C2	1.747 (2)
N1—S2	1.7198 (14)	C3—O5	1.192 (2)
S1—O1	1.4191 (13)	C3—C4	1.535 (2)
S1—O2	1.4305 (12)	C4—O6	1.177 (2)
S1—C1	1.745 (2)	C4—Cl	1.734 (2)
S2—O3	1.4140 (13)		
C3—N1—S1	119.51 (11)	N1—C3—C4	115.40 (13)
C3—N1—S2	117.78 (10)	O6—C4—C3	124.1 (2)
S1—N1—S2	120.77 (7)	O6—C4—Cl	123.85 (14)
O5—C3—N1	123.8 (2)	C3—C4—Cl	111.66 (12)
O5—C3—C4	120.40 (15)		

Table 2. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···O4$^{\rm i}$	0.98	2.58	3.338 (2)	134.3
C2—H2*A*···O4$^{\rm ii}$	0.98	2.65	3.289 (2)	122.9
C2—H2*B*···O1$^{\rm iii}$	0.98	2.56	3.440 (2)	150.0
C2—H2*C*···O5$^{\rm iv}$	0.98	2.60	3.377 (2)	136.8

Symmetry codes: (i) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$; (ii) $\frac{1}{2} + x, \frac{3}{2} - y, 1 - z$; (iii) $\frac{3}{2} - x, 1 - y, \frac{1}{2} + z$; (iv) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$.

Data collection: *DIF*4 (Stoe & Cie, 1991*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1991*b*). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *XP* (Siemens, 1994). Software used to prepare material for publication: *SHELXL*93.

The authors thank the Fonds der Chemischen Industrie for financial support and Mr A. Weinkauf for technical assistance.

Lists of atomic coordinates, displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: FG1267). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–S19.
Blaschette, A., Dalluhn, J., Fischer, A. & Jones, P. G. (1994). *Z. Kristallogr.* **209**, 445–447.
Blaschette, A., Linoh, K., Koch, D. & Ernst, L. (1989). *Z. Naturforsch. Teil B*, **44**, 465–474.
Dalluhn, J. (1995). PhD thesis, Technical University of Braunschweig, Germany. [ISBN 3-931443-04-3]
Dalluhn, J., Pröhl, H.-H., Blaschette, A., Lange, I. & Jones, P. G. (1994). *Phosphorus Sulfur Silicon*, **89**, 69–76.
Dalluhn, J., Pröhl, H.-H., Henschel, D., Blaschette, A. & Jones, P. G. (1996). *Phosphorus Sulfur Silicon*, **114**, 149–160.
Desiraju, G. R. (1996). *Acc. Chem. Res.* **29**, 441–449.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Groth, P. & Hassel, O. (1962). *Acta Chem. Scand.* **16**, 2311–2317.
Hagen, K. & Hedberg, K. (1973). *J. Am. Chem. Soc.* **95**, 1003–1009.
Jones, P. G., Hamann, T., Schaper, W., Lange, I. & Blaschette, A. (1995). *Phosphorus Sulfur Silicon*, **106**, 91–104.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures.* University of Göttingen, Germany.
Siemens (1994). *XP. Interactive Molecular Graphics Program.* Version 5.03. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Stoe & Cie (1991*a*). *DIF4. Diffractometer Control Program.* Version 7.08. Stoe & Cie, Darmstadt, Germany.
Stoe & Cie (1991*b*). *REDU4. Data Reduction Program.* Version 7.08. Stoe & Cie, Darmstadt, Germany.
Wirth, A., Henschel, D., Blaschette, A. & Jones, P. G. (1997). *Z. Anorg. Allg. Chem.* In the press.
Yamaguchi, K., Matsumura, G., Haga, N. & Shudo, K. (1992). *Acta Cryst.* C**48**, 558–559.

Acta Cryst. (1997). C**53**, 783–786

2,4,6-Tris(diazo)cyclohexane-1,3,5-trione

PETER G. JONES,[a] BIRTE AHRENS,[a] THOMAS HÖPFNER[b] AND HENNING HOPF[b]

[a]*Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Postfach 3329, 38023 Braunschweig, Germany, and* [b]*Institut für Organische Chemie, Technische Universität Braunschweig, Postfach 3329, 38023 Braunschweig, Germany. E-mail: jones@xray36.anchem.nat.tu-bs.de*

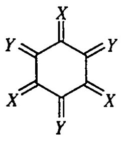
(*Received 17 December 1996; accepted 3 February 1997*)

Abstract

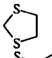
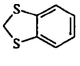
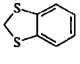
The title compound, $C_6N_6O_3$, displays crystallographic $\bar{6}$ symmetry. All atoms lie in mirror planes. The actual symmetry is close to the ideal $\bar{6}m2$. Ring angles alternate between 112.37 (9)° at the keto and 127.63 (9)° at the diazo C atoms. The molecules form layers with hexagonal close packing.

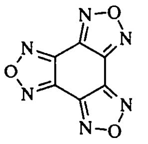
Comment

As part of our current investigations on cross-conjugated π systems, we were interested in the structure of the hetero[6]radialene 2,4,6-tris(diazo)cyclohexane-1,3,5-trione, (1*a*) (for reviews on radialenes see Hopf & Maas, 1992*a*,*b*, 1997). Past X-ray structural investigations have shown that fully or partially bridged systems such as (2) (Cameron & Prout, 1972), (3) (Kono *et al.*, 1989*a*,*b*; Otsubo *et al.*, 1993) and (4) (Kabuto, Suzuki, Yamashita & Mukai, 1986; Suzuki *et al.*, 1987, 1992; Suzuki, Fukushima, Yamashita & Miyashi, 1994; Suzuki, Kabuto, Yamashita, Mukai & Miyashi, 1988; Yamashita *et al.*, 1993; Yamashita, Tanaka, Imaeda & Inokuchi, 1991; Yamashita, Tanaka, Imaeda, Inokuchi & Sano, 1992) possess planar six-membered rings, whereas the cyclohexane moieties of unbridged derivatives such as (1*c*) (Marsh & Dunitz, 1975), (1*d*) (Wilke, 1988*a*,*b*) and (1*f*) (Sugimoto *et al.*, 1987) usually adopt non-planar conformations. Exceptions are (5) (Ansell, 1969) which is closely related to the title compound, and (1*e*), in which the planar ring is associated with short (shorter than van der Waals) interactions between the O and S atoms (Kimura, Watson & Nakayama, 1980; Coffin, Bryce & Clegg, 1992).

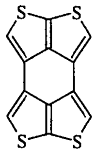


(1)

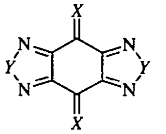
	X	*Y*
(*a*)	O	N_2
(*b*)	CH_2	CH_2
(*c*)	$CHCH_3$	$CHCH_3$
(*d*)	$C(CH_3)_2$	$C(CH_3)_2$
(*e*)	O	
(*f*)		



(2)

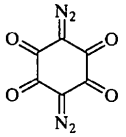


(3)



(4)

	X	*Y*
(*a*)	$C(CN)_2$	S
(*b*)	$C(CN)_2$	Se



(5)

From these comparisons, it can be concluded that the conformation of the cyclohexane moiety in unbridged [6]radialenes is determined by the steric requirements of their exocyclic substituents. Even methylene groups seem to be 'large' in this respect, as was shown by *ab initio* calculations on (1*b*), which predicted the six-membered ring would adopt a chair conformation (Benet-Buchholz, Boese, Hauman & Traetteberg, 1997).

The molecule of (1*a*) is shown in Fig. 1. All atoms lie in the mirror plane $z = 0.25$ (and symmetry-equivalent molecules at $z = 0.75$) and the crystallographic symmetry is $3/m$ ($\bar{6}$), although the actual symmetry is close to the ideal $\bar{6}m2$. The ring angles alternate between 112.37 (9) at C1 (C=O) and 127.63 (9)° at C2 (C=N=N). In studies of *p*-benzoquinone diazides (Sander *et al.*, 1993), we were able to show that ring angles at C=O were less than, and at C=N=N greater than, 120°, although not as markedly as in (1*a*). Ring bond lengths in (1*a*) are essentially equal. The bond lengths involving the substituents [C1—O 1.2278 (11), C2—N1 1.3311 (12) and N1—N2 1.1077 (12) Å] correspond to the lower range of those observed for the *p*-benzoquinone diazides.

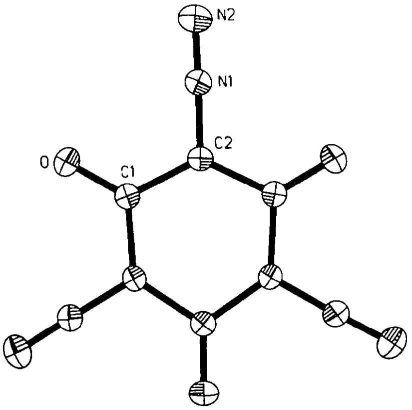


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Only the asymmetric unit is numbered.

The packing diagram (Fig. 2) shows a hexagonal close packing (layer sequence *ABAB*). The interlayer separation is $c/2$ = 2.723 (2) Å. The shortest interatomic contact between layers is N1···O($x-y$, x, $-z$) 3.003 (1) Å.

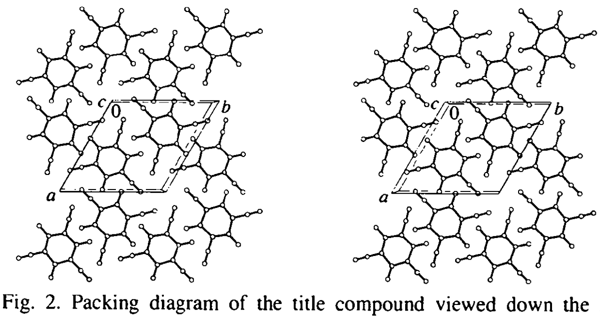


Fig. 2. Packing diagram of the title compound viewed down the z axis.

Experimental

The planar hetero[6]radialene (1*a*) was obtained according to the procedure of Ried & Mengler (1965). Spectroscopic data: ^{13}C NMR (CD$_2$Cl$_2$, Bruker AM 400): δ 170.74 (C=O), 81.21 (C=N); IR (KBr, Nicolet FT-IR 320), ν: 2474 (*w*), 2227 (*w*), 2192 (*m*), 2145 (*s*), 1662 (*w*), 1608 (*s*), 1582 (*w*), 1571 (*w*), 1393 (*m*), 1383 (*m*), 1353 (*s*), 1307 (*w*), 1219 (*m*), 972 (*m*), 750 (*m*), 404 (*w*); UV/Vis (CH_3CN, HP 8452 A Diode Array Spectrophotometer), $\lambda_{\max}$ (log ε): 226 (4.307), 254 (4.670); MS (EI, Finnigan MAT 8430), *m*/*z* (%): 205 (8), 204 (100) [M^+]. Slow evaporation of a CD_2Cl_2 solution yielded crystals of X-ray diffraction quality.

Crystal data

$C_6N_6O_3$
$M_r = 204.12$
Hexagonal
$P6_3/m$
$a = 9.1599\,(13)$ Å
$c = 5.445\,(3)$ Å
$V = 395.6\,(2)$ Å^3
$Z = 2$
$D_x = 1.713$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 60 reflections
$\theta = 10.0–11.5°$
$\mu = 0.144$ mm^{-1}
$T = 143\,(2)$ K
Prism
0.75 × 0.60 × 0.40 mm
Pale yellow

Data collection

Stoe Stadi-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2386 measured reflections
408 independent reflections
385 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.0516$

$\theta_{\max} = 29.45°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -7 \rightarrow 7$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0291$
$wR(F^2) = 0.0933$
$S = 1.184$
407 reflections
32 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.0293P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.410$ e Å^{-3}
$\Delta\rho_{\min} = -0.187$ e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.70 (6)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
O	0.41446 (9)	0.00385 (9)	1/4	0.0249 (3)
N1	0.33774 (11)	0.25478 (10)	1/4	0.0226 (3)
N2	0.20295 (12)	0.21895 (13)	1/4	0.0331 (3)
C1	0.52808 (12)	0.15168 (12)	1/4	0.0196 (3)
C2	0.49860 (11)	0.29383 (12)	1/4	0.0207 (3)

Table 2. *Selected geometric parameters (Å, °)*

O—C1	1.2278 (11)	C1—C2$^{\rm i}$	1.4506 (12)
N1—N2	1.1077 (12)	C1—C2	1.4560 (12)
N1—C2	1.3311 (12)		
N2—N1—C2	178.59 (10)	N1—C2—C1$^{\rm ii}$	116.58 (8)
O—C1—C2$^{\rm i}$	124.11 (8)	N1—C2—C1	115.79 (9)
O—C1—C2	123.52 (8)	C1$^{\rm ii}$—C2—C1	127.63 (9)
C2$^{\rm i}$—C1—C2	112.37 (9)		

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

Data collection: *DIF*4 (Stoe & Cie, 1991*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1991*b*). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *XP* (Siemens, 1994). Software used to prepare material for publication: *SHELXL*93.

The authors thank the Volkswagen-Stiftung, the Cusanuswerk and the Fonds der Chemischen Industrie for financial support and Mr A. Weinkauf for technical assistance.

Lists of atomic coordinates, displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: FG1274). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Ansell, G. B. (1969). *J. Chem. Soc. B*, pp. 729–732.
Benet-Buchholz, J., Boese, R., Hauman, T. & Traetteberg, M. (1997). In *Structural Chemistry of Polyenes*, edited by S. Patai. Chichester, New York, Brisbane, Toronto: John Wiley & Sons. In the press.
Cameron, T. S. & Prout, C. K. (1972). *Acta Cryst.* B**28**, 447–452.
Coffin, M. A., Bryce, M. R. & Clegg, W. (1992). *J. Chem. Soc. Chem. Commun.* pp. 401–402.
Hopf, H. & Maas, G. (1992*a*). *Angew. Chem.* **104**, 953–977.
Hopf, H. & Maas, G. (1992*b*). *Angew. Chem. Int. Ed. Engl.* **31**, 931–954.
Hopf, H. & Maas, G. (1997). *The Chemistry of Dienes and Polyenes*, Vol. 1, edited by T. Rappaport, pp. 927–977. Chichester: John Wiley & Sons.
Kabuto, C., Suzuki, T., Yamashita, Y. & Mukai, T. (1986). *Chem. Lett.* pp. 1433–1436.
Kimura, M., Watson, W. H. & Nakayama, J. (1980). *J. Org. Chem.* **45**, 3719–3721.
Kono, Y., Miyamoto, H., Aso, Y., Otsubo, T., Ogura, F., Tanaka, T. & Sawada, M. (1989*a*). *Angew. Chem.* **101**, 1254–1255.
Kono, Y., Miyamoto, H., Aso, Y., Otsubo, T., Ogura, F., Tanaka, T. & Sawada, M. (1989*b*). *Angew. Chem. Int. Ed. Engl.* **28**, 1222–1223.
Marsh, W. & Dunitz, J. D. (1975). *Helv. Chim. Acta*, **58**, 707–712.
Otsubo, T., Kono, Y., Hozo, N., Miyamoto, H., Aso, Y., Ogura, F., Tanaka, T. & Sawada, M. (1993). *Bull. Chem. Soc. Jpn*, **66**, 2033–2041.
Ried, W. & Mengler, H. (1965). *Fortschritte der Chemischen Forschung*, Vol. 5/1, pp. 1–88. Heidelberg: Springer.
Sander, W., Bucher, G., Komnick, P., Morawietz, J., Bubenitschek, P., Jones, P. G. & Chrapkowski, A. (1993). *Chem. Ber.* **126**, 2101–2109.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures.* University of Göttingen, Germany.
Siemens (1994). *XP. Interactive Molecular Graphics Program.* Version 5.03. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Stoe & Cie (1991*a*). *DIF4. Diffractometer Control Program.* Version 7.08. Stoe & Cie, Darmstadt, Germany.
Stoe & Cie (1991*b*). *REDU4. Data Reduction Program.* Version 7.08. Stoe & Cie, Darmstadt, Germany.
Sugimoto, T., Misaki, Y., Kajita, T., Yoshida, Z.-I., Kai, Y. & Kasai, N. (1987). *J. Am. Chem. Soc.* **109**, 4106–4107.
Suzuki, T., Fujii, H., Yamashita, Y., Kabuto, C., Tanaka, S., Harasawa, M., Mukai, T. & Miyashi, T. (1992). *J. Am. Chem. Soc.* **114**, 3034–3043.
Suzuki, T., Fukushima, T., Yamashita, Y. & Miyashi, T. (1994). *J. Am. Chem. Soc.* **116**, 2793–2803.

Suzuki, T., Kabuto, C., Yamashita, Y., Mukai, T. & Miyashi, T. (1988). *J. Chem. Soc. Chem. Commun.* pp. 895–896.
Suzuki, T., Kabuto, C., Yamashita, Y., Saito, G., Mukai, T. & Miyashi, T. (1987). *Chem. Lett.* pp. 2285–2288.
Wilke, D. (1988*a*). *Angew. Chem.* **100**, 189–211.
Wilke, D. (1988*b*). *Angew. Chem. Int. Ed. Engl.* **27**, 185–206.
Yamashita, Y., Ono, K., Tanaka, S., Imaeda, K., Inokuchi, H. & Sano, M. (1993). *J. Chem. Soc. Chem. Commun.* pp. 1803–1805.
Yamashita, Y., Tanaka, S., Imaeda, K. & Inokuchi, H. (1991). *Chem. Lett.* pp. 1213–1216.
Yamashita, Y., Tanaka, S., Imaeda, K., Inokuchi, H. & Sano, M. (1992). *J. Org. Chem.* **57**, 5517–5522.

Acta Cryst. (1997). C**53**, 786–787

2,13-Dithia[3]orthocyclo[3](2,3)-naphthalenophane†

Peter G. Jones[a] and Piotr Kuś[b]

[a]*Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Postfach 3329, 38023 Braunschweig, Germany, and* [b]*Department of Chemistry, Silesian University, 9 Szkolna Street, 40-006 Katowice, Poland. E-mail: jones@xray36.anchem.nat.tu-bs.de*

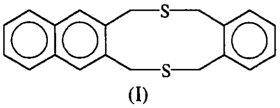
(*Received 30 September 1996; accepted 2 January 1997*)

Abstract

The title compound, $C_{20}H_{18}S_2$, crystallizes with two independent but closely similar molecules in the asymmetric unit. The aromatic ring systems are parallel and adopt the *anti* conformation.

Comment

We are interested in structures, particularly conformational aspects, of cyclophane systems (see, for example, Bodwell, Ernst, Hopf & Jones, 1989; Jones, Hopf & Kuś, 1996). We present here the structure of the sulfur-containing cyclophane 2,13-dithia[3]orthocyclo[3](2,3)-naphthalenophane, (I).



(I)

The title compound crystallizes with two molecules in the asymmetric unit (Fig. 1), which are, however, closely similar; a least-squares fit (molecule 2 inverted) showed a mean deviation of 0.07 Å.

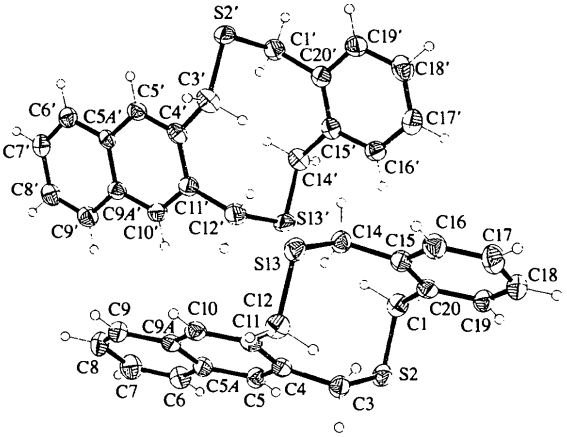


Fig. 1. Both independent molecules of the title compound in the crystal. Ellipsoids represent 50% probability levels and H-atom radii are arbitrary.

The aromatic ring systems in each molecule are almost parallel [interplanar angles of 1.4 (1) and 2.5 (1)°] and adopt the *anti* conformation, as previously observed by us in the closely related structure 2,11-dithia-[3.3](5,6)indanoorthocyclophane (Bodwell *et al.*, 1989) and by Okajima, Wang & Fukazawa (1989) in the parent compound 2,11-dithia[3.3]orthocyclophane, which displays inversion symmetry. The perpendicular distance between the ring systems (as given by the deviations of atoms C15–C20 and C15′–C20′ from the naphthalene best plane) is *ca* 2.4–2.5 Å.

Bond lengths, angles and torsion angles of the central ten-membered rings are given in Table 1. Starting with C1—S2—C3—C4 and moving to increasing atom number, the torsion angle sequence is +*sc*, −*sc*, *sp*, +*ac*, −*ac*, −*ac*, +*ac*, *sp*, −*sc*, +*sc* in molecule 1 (and in molecule 2 when inverted), as previously observed by Bodwell *et al.* (1989).

Experimental

The title compound was prepared as reported by Kuś (1987) and recrystallized from dichloromethane/*n*-butanol.

Crystal data

$C_{20}H_{18}S_2$
$M_r = 322.46$
Triclinic
$P\bar{1}$
$a = 10.646\,(3)$ Å
$b = 11.286\,(3)$ Å
$c = 14.205\,(4)$ Å
$\alpha = 78.20\,(2)°$
$\beta = 80.64\,(2)°$
$\gamma = 71.77\,(2)°$
$V = 1577.9\,(8)$ Å^3
$Z = 4$
$D_x = 1.357$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 50 reflections
$\theta = 10.0–11.5°$
$\mu = 0.331$ mm^{-1}
$T = 143\,(2)$ K
Prism
0.80 × 0.20 × 0.20 mm
Colourless

---

† Alternative name: 3,12-dithiatetracyclo[12.8.0.0^{5,12}.0^{16,21}]docosane-5,7,9,14,16,18,20,22-octaene.

Acta Crystallographica Section C
ISSN 0108-2701 © 1997