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#### Key indicators

Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$   
R factor = 0.050  
wR factor = 0.142  
Data-to-parameter ratio = 17.6

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

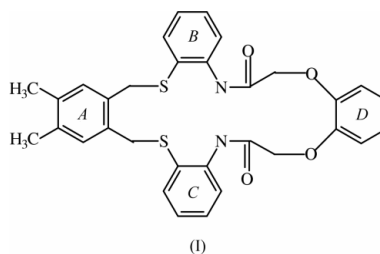
## 34,35-Dimethyl-13,20-dioxa-10,23-diaza-3,30-dithiapentacyclo[30.4.0.0<sup>4,9</sup>.0<sup>14,19</sup>.0<sup>24,29</sup>]hexatriconta-1(36),4,6,8,14,16,18,24,26,28,32,34-dodecane-11,22-dione

The structure of the title molecule,  $\text{C}_{32}\text{H}_{30}\text{N}_2\text{O}_4\text{S}_2$ , is stabilized by  $\text{N}-\text{H}\cdots\text{O}$ ,  $\text{N}-\text{H}\cdots\text{S}$ ,  $\text{C}-\text{H}\cdots\text{S}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds. The molecular packing in the crystal is stabilized by intermolecular  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\pi$  interactions.

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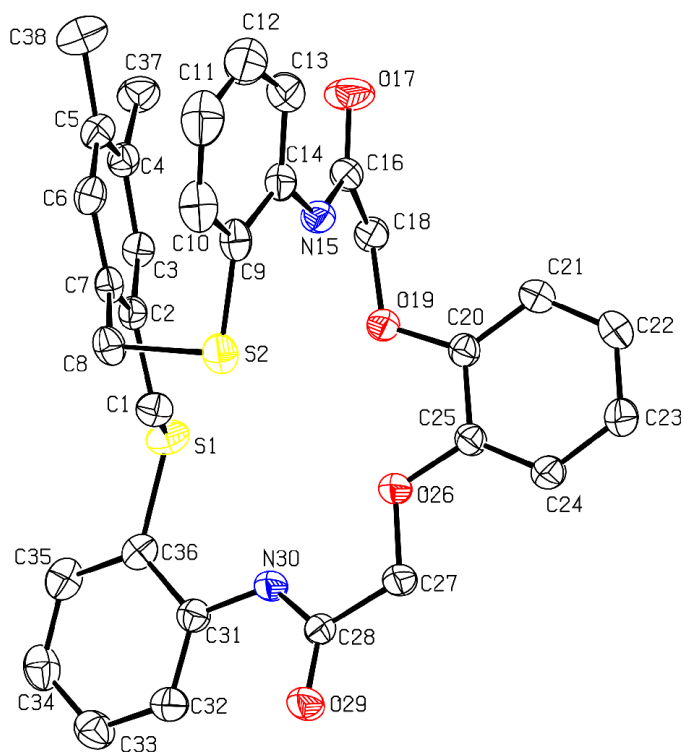
### Comment

Cyclophanes are cyclic systems, consisting of at least one aromatic moiety, bridged by one or more aliphatic chains (De Ridder *et al.*, 2001). Paracyclophane and other  $\pi$ -electron-rich hydrocarbons possessing a cavity-forming topology are known to form endohedral  $\pi$ -complexes with silver and other soft metal atoms (Addad *et al.*, 1983; Heirtzler *et al.*, 1995; Faust, 1995). We report here the structure of the title compound, (I), a cyclophane.

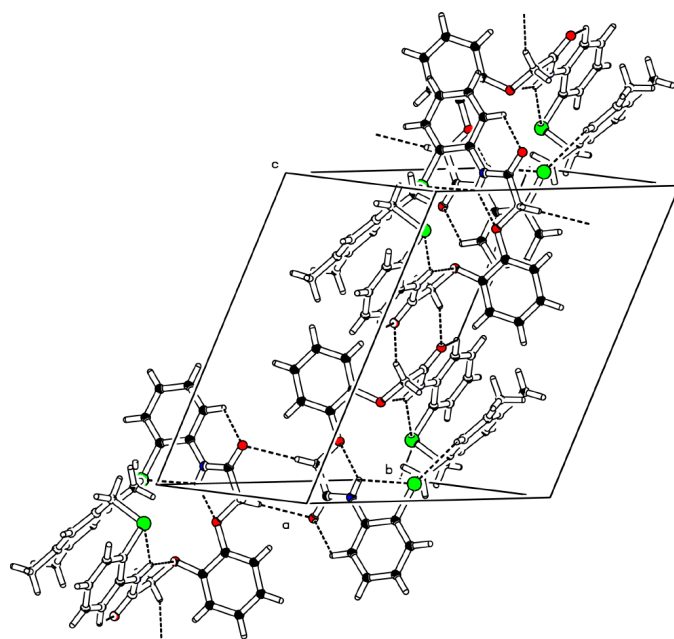


The structure of (I) with the atom-numbering scheme is shown in Fig. 1. The  $\text{S}-\text{C}$  distances [ $\text{S}1-\text{C}36 = 1.774 (2) \text{ \AA}$ ,  $\text{S}1-\text{C}1 = 1.821 (2) \text{ \AA}$ ,  $\text{S}2-\text{C}9 = 1.772 (2) \text{ \AA}$  and  $\text{S}2-\text{C}8 = 1.844 (2) \text{ \AA}$ ] are comparable to the mean  $\text{C}_{\text{phenyl}}-\text{S}$  [ $1.773 (9) \text{ \AA}$ ] or  $\text{Csp}^3-\text{S}$  [ $1.819 (19) \text{ \AA}$ ] distances reported by Allen *et al.* (1987). The widening of the exocyclic angle  $\text{C}24-\text{C}25-\text{O}26$  [ $124.8 (2)^\circ$ ] and the resultant narrowing of angle  $\text{C}20-\text{C}25-\text{O}26$  [ $114.8 (2)^\circ$ ] from  $120^\circ$  may be a result of the short  $\text{H}24\cdots\text{H}27\text{B}$  [ $2.13 \text{ \AA}$ ] contact. The torsion angles  $\text{C}13-\text{C}14-\text{N}15-\text{C}16 = -15.4 (3)^\circ$ ,  $\text{C}9-\text{C}14-\text{N}15-\text{C}16 = 163.8 (2)^\circ$ ,  $\text{C}36-\text{C}31-\text{N}30-\text{C}28 = 162.5 (2)^\circ$  and  $\text{C}28-\text{N}30-\text{C}31-\text{C}32 = -19.0 (3)^\circ$  indicate that both the amide planes are twisted away from the attached benzene rings; the dihedral angle between the  $\text{N}15/\text{C}16/\text{O}17/\text{C}18$  plane and ring *B* is  $13.3 (1)^\circ$  and that between  $\text{N}30/\text{C}28/\text{O}29/\text{C}27$  plane and ring *C* is  $17.2 (1)^\circ$ . The dihedral angle between the benzene rings *A* and *D* [ $87.3 (1)^\circ$ ] and *B* and *C* [ $86.4 (1)^\circ$ ] indicate that they are nearly perpendicular to each other.

The molecular structure is stabilized by  $\text{N}-\text{H}\cdots\text{O}$ ,  $\text{N}-\text{H}\cdots\text{S}$ ,  $\text{C}-\text{H}\cdots\text{S}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds. In the crystal structure,  $\text{C}18-\text{H}18\text{B}\cdots\text{O}17^i$  hydrogen bonds link inversion-related molecules to form dimers (Fig. 2). The dimers are linked together by  $\text{C}27-\text{H}27\text{B}\cdots\text{O}29^{ii}$  hydrogen



**Figure 1**  
The molecular structure of the title compound, showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity.



**Figure 2**  
A view of the molecular packing.

bonds (Table 1). The structure is further stabilized by intermolecular C—H $\cdots$  $\pi$  interactions involving H37B and ring D of the molecule translated by a unit along the *a* axis [H37B $\cdots$ CgD = 2.79 Å, C37 $\cdots$ CgD 3.638 (3) Å and C37—H37B $\cdots$ CgD = 148°, where CgD is the centroid of ring D in the translated molecule].

## Experimental

In high dilution condition, benzene-1,2-dioxy-bis(ethanoylchloride) (1 mmol) and 1,2-dimethyl-4,5-bis[mercaptomethyl(2-amino-phenyl)]benzene (1 mmol) were cyclized in chloroform in the presence of triethylamine to afford the title compound. The compound was recrystallized by slow evaporation from a chloroform/hexane (1:1) mixture.

### Crystal data

C<sub>32</sub>H<sub>30</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub>  
*M<sub>r</sub>* = 570.70  
 Triclinic, *P*1  
*a* = 8.5860 (7) Å  
*b* = 12.9090 (10) Å  
*c* = 14.7552 (11) Å  
 $\alpha$  = 65.065 (1)°  
 $\beta$  = 84.701 (1)°  
 $\gamma$  = 76.522 (1)°  
*V* = 1442.1 (2) Å<sup>3</sup>

*Z* = 2  
*D<sub>x</sub>* = 1.314 Mg m<sup>-3</sup>  
 Mo *K* $\alpha$  radiation  
 Cell parameters from 2732 reflections  
 $\theta$  = 2.7–26.3°  
 $\mu$  = 0.23 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Needle, colourless  
 0.25 × 0.19 × 0.14 mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: none  
 9187 measured reflections  
 6389 independent reflections

4720 reflections with *I* > 2 $\sigma$ (*I*)  
*R*<sub>int</sub> = 0.017  
 $\theta$ <sub>max</sub> = 28.0°  
*h* = -10 → 11  
*k* = -17 → 13  
*l* = -19 → 18

### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.050  
*wR*(*F*<sup>2</sup>) = 0.142  
*S* = 1.01  
 6389 reflections  
 363 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2 + 0.1322P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.27 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.19 \text{ e \AA}^{-3}$

**Table 1**

Hydrogen-bonding 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>
N15—H15 $\cdots$ S2	0.86	2.57	3.012 (2)	113
N15—H15 $\cdots$ O19	0.86	2.22	2.681 (2)	114
N30—H30 $\cdots$ S1	0.86	2.55	2.999 (2)	113
N30—H30 $\cdots$ O26	0.86	2.18	2.618 (2)	111
C3—H3 $\cdots$ S1	0.93	2.56	3.029 (2)	112
C13—H13 $\cdots$ O17	0.93	2.33	2.904 (4)	120
C32—H32 $\cdots$ O29	0.93	2.31	2.884 (3)	119
C18—H18B $\cdots$ O17 <sup>i</sup>	0.97	2.39	3.300 (3)	157
C27—H27B $\cdots$ O29 <sup>ii</sup>	0.97	2.47	3.398 (3)	161

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

H atoms were positioned geometrically and were treated as riding on their parent atoms, with C—H (aromatic) = 0.93 Å, C—H (methyl) = 0.96 Å, C—H (methylene) = 0.97 Å and N—H = 0.86 Å. *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(C) for methyl H and 1.2*U*<sub>eq</sub>(C or N) for other H atoms. A rotating-group model was used for the methyl groups. Reflections were measured to  $\theta_{\max}$  = 28.0° with 92% completeness, but the data are 99% complete to 25°.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 1990); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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