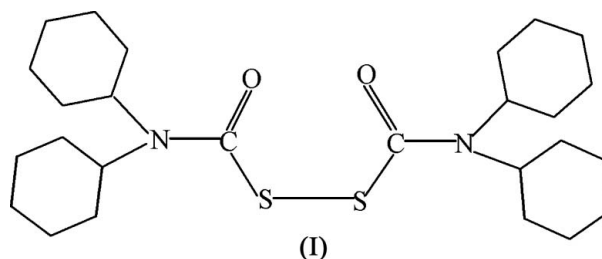


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Key indicators

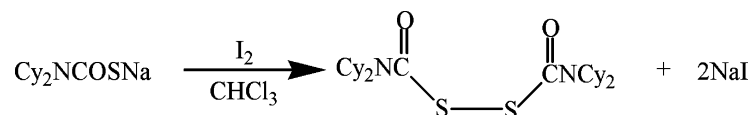
Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.047
 wR factor = 0.127
Data-to-parameter ratio = 16.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis(*N,N*-dicyclohexylthiocarbamoyl) disulfideThe title compound, $\text{C}_{26}\text{H}_{44}\text{N}_2\text{S}_2$, was prepared by the oxidation of the corresponding thiocarbamate with iodine. The disulfide S—S distance is close to the distances observed in free (uncoordinated) disulfides. A crystallographic twofold axis passes through the mid-point of the S—S bond.Received 18 November 2005
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Comment

The reaction of I_2 with *N,N*-dicyclohexylcarbamate produced the title compound, (I), the synthesis and structure of which is reported here. The molecular structure is shown in Fig. 1. Selected bond lengths and angles are listed in Table 1. In (I), the C—S and C—O distances are consistent with single and double bond lengths, respectively. A crystallographic twofold axis passes through the mid-point of the S—S bond.The disulfide S—S distance is close to the distances observed in free (uncoordinated) disulfides (Kumar *et al.*, 1990). The $\text{C}_{\text{sp}^2}\text{—N}$ bond distance observed in this complex is similar to that observed in analogous compounds, confirming the considerable double-bond character associated with these bonds.

Experimental

Iodine (1 mmol) in chloroform (50 ml) was added dropwise to a solution containing dicyclohexylcarbamate (1 mmol) in chloroform (20 ml) over a period of 2 h with continuous stirring.

Light turbidity appeared in the solution after 30 min, which was removed by filtration. The filtrate was left undisturbed at room temperature. After 2 d, pale-yellow crystals formed. The crystals were filtered off, washed with chloroform and then dried [m.p. 468 K (decomposition)]. Analysis calculated (%) for $\text{C}_{26}\text{H}_{44}\text{N}_2\text{O}_2\text{S}_2$: C 64.95, H 9.22, N 5.83; found: C 64.72, H 9.38, N 6.01.

Crystal data

C₂₆H₄₄N₂O₂S₂
 M_r = 480.75
 Monoclinic, C2/c
 a = 12.868 (3) Å
 b = 25.435 (6) Å
 c = 9.080 (2) Å
 β = 116.579 (3)°
 V = 2657.8 (11) Å³
 Z = 4

D_x = 1.201 Mg m⁻³
 Mo Kα radiation
 Cell parameters from 1510 reflections
 θ = 2.5–24.3°
 μ = 0.23 mm⁻¹
 T = 298 (2) K
 Block, yellow
 0.53 × 0.41 × 0.32 mm

Data collection

Siemens SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 T_{min} = 0.890, T_{max} = 0.932
 6913 measured reflections

2341 independent reflections
 1519 reflections with I > 2σ(I)
 R_{int} = 0.050
 θ_{max} = 25.0°
 h = -15 → 14
 k = -24 → 30
 l = -10 → 10

Refinement

Refinement on F²
 R[F² > 2σ(F²)] = 0.047
 wR(F²) = 0.127
 S = 1.00
 2341 reflections
 145 parameters
 H-atom parameters constrained

w = 1/[σ²(F_o²) + (0.0586P)² + 1.1207P]
 where P = (F_o² + 2F_c²)/3
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.37 e Å⁻³
 Δρ_{min} = -0.19 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

S1–C1	1.849 (3)	N1–C8	1.475 (3)
S1–S1 ⁱ	2.0138 (13)	N1–C2	1.488 (3)
N1–C1	1.350 (3)	O1–C1	1.227 (3)
C1–S1–S1 ⁱ	100.35 (9)	O1–C1–S1	119.5 (2)
C1–N1–C8	123.0 (2)	N1–C1–S1	113.98 (19)
C1–N1–C2	118.7 (2)	N1–C2–C3	113.3 (2)
C8–N1–C2	117.9 (2)	N1–C2–C7	112.7 (2)
O1–C1–N1	126.5 (2)		

Symmetry code: (i) -x + 1, y, -z + ½.

All H atoms were positioned geometrically and refined as riding on their parent atoms, with methylene C–H distances of 0.97 Å and other C–H = 0.98 Å, U_{iso}(H) = 1.2U_{eq}(C).

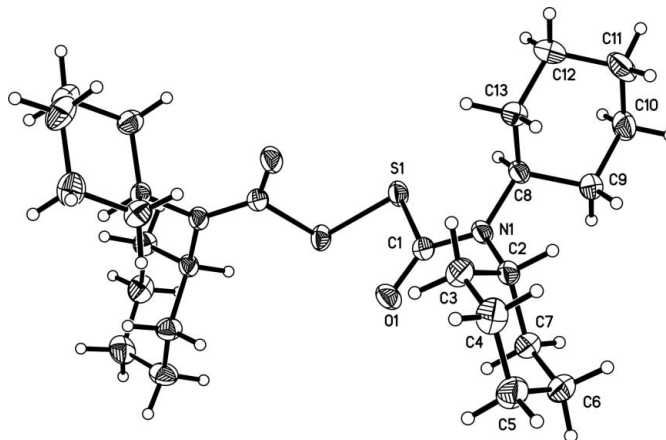


Figure 1

The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering schemes (symmetry code for unlabelled atoms: -x + 1, y, -z + ½).

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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