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(1*E*)-5-Amino-1,5-bis[4-(methylsulfanyl)-phenyl]pent-1-en-3-one

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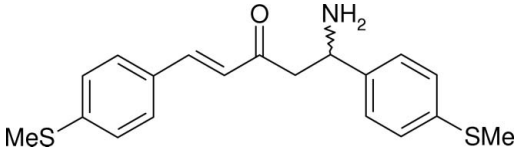
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.053; wR factor = 0.149; data-to-parameter ratio = 14.1.

The title compound, $C_{19}H_{21}NOS_2$, arose as an unexpected product in a bis-chalcone synthesis. The dihedral angle between the two ring planes is 31.87 (14)°. Both terminal methyl groups are disordered over two positions each; the site occupancy ratios are 0.56:0.44 and 0.65:0.35. In the crystal structure, adjacent molecules are linked into $C(2)$ chains propagating along [010] by way of N—H···N hydrogen bonds.

Related literature

For related structures, see: Butcher, Yathirajan, Sarojini, Narayana & Indira (2006); Butcher, Yathirajan, Sarojini, Narayana & Vijaya Raj (2006); Harrison *et al.* (2006); Etter (1990).



Experimental

Crystal data

$C_{19}H_{21}NOS_2$
M_r = 343.49
Orthorhombic, *Pbca*
a = 16.705 (3) Å
b = 5.5968 (10) Å
c = 37.730 (7) Å
V = 3527.5 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 295 (2) K
0.40 × 0.20 × 0.05 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.888, T_{max} = 0.986
17587 measured reflections
3278 independent reflections
1465 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.149
S = 0.91
3278 reflections
232 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···N1^{i}	0.89	2.22	3.0981 (19)	167

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); 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); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2020).

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supplementary materials

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(1*E*)-5-Amino-1,5-bis[4-(methylsulfanyl)phenyl]pent-1-en-3-one

W. T. A. Harrison, B. K. Sarojini, S. Bindya, B. Narayana and H. S. Yathirajan

Comment

As part of our ongoing studies Butcher, Yathirajan, Sarojini, Narayana & Indira, 2006; Butcher, Yathirajan, Sarojini, Narayana & Vijaya Raj, 2006; Harrison *et al.*, 2006) of the syntheses and structures of chalcone derivatives, the title compound, (I), (Fig. 1) is described here. It arose as an unexpected product from an attempt to prepare the symmetric methylthio-substituted bis-chalcone 1,5-di(4-methylthiophenyl)penta-1,4-dien-3-one.

The dihedral angle between the mean planes of the aromatic rings in (I) is 31.87 (14)°. The molecule of (I) is chiral. In the arbitrarily chose asymmetric molecule, C11 has *R* configuration, but crystal symmetry generates a racemic mixture.

In the crystal, adjacent molecules of (I) interact by way of N—H···N hydrogen bonds (Table 1) to result in C(2) chains (Etter, 1990) propagating in [010] (Fig. 2).

Experimental

A solution of 25 ml of NH_3 in 150 ml of water and 100 ml of ethanol was placed in a 500-ml bolt-head flask provided with a mechanical stirrer. The flask was immersed in a water bath and the temperature of the solution was maintained at 393–398 K. The solution was vigorously stirred and one half of a previously prepared mixture of 4-(methylthio)benzaldehyde (38 g, 0.25 mol) and acetone (7.3 g, 0.125 mol) was added. A flocculent precipitate was formed within 2–3 minutes. After 15 minutes, the remainder of the aldehyde-acetone mixture was added and the stirring was continued for a further 40 minutes. The crude product obtained was filtered and washed with cold water to eliminate the alkali (yield: 70%). The compound was purified from ethanol-dioxane mixture (8:2 *v*/*v*). The crystal growth was done in acetone:toluene (1:1 *v*/*v*) by slow evaporation to yield amber plates and slabs of (I) (m.p. 348–353 K).

Refinement

Both terminal methyl groups are disordered over two positions, with occupancies of 0.557 (10):0.443 (10) for C18A/C18B and 0.642 (9):0.358 (9) for C19A/C19B (occupancy sums constrained to unity in both cases).

The hydrogen atoms were geometrically placed (C—H = 0.93–0.98 Å, N—H = 0.89 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C,*N*) or 1.5U_{eq}(methyl C).

Figures

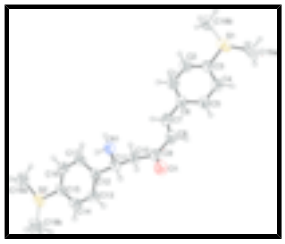

Fig. 1. View of the molecular structure of (I) showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). One disorder component for each terminal methyl group is bonded to its S atom with a dashed line.

Fig. 2. A fragment of an [010] hydrogen-bonded chain in the crystal of (I). The H bonds are shown as double dashed lines. All C-bound H atoms and one methyl disorder component are omitted for clarity. Symmetry code as in Table 1.

(1E)-5-Amino-1,5-bis[4-(methylsulfanyl)phenyl]pent-1-en-3-one

Crystal data

$C_{19}H_{21}NOS_2$	F_{000} = 1456
M_r = 343.49	D_x = 1.294 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 723 reflections
a = 16.705 (3) Å	θ = 4.4–23.3º
b = 5.5968 (10) Å	μ = 0.31 mm^{-1}
c = 37.730 (7) Å	*T* = 295 (2) K
V = 3527.5 (11) Å^3	Slab, orange
Z = 8	0.40 × 0.20 × 0.05 mm

Data collection

Bruker SMART 1000 CCD diffractometer	3278 independent reflections
Radiation source: fine-focus sealed tube	1465 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.073
T = 295(2) K	θ_{max} = 25.5º

ω scans	θ_{min} = 4.3°
Absorption correction: multi-scan (SADABS; Bruker, 1999)	h = −20→19
T_{min} = 0.888, T_{max} = 0.986	k = −6→6
17587 measured reflections	l = −45→43

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H-atom parameters constrained
$wR(F^2)$ = 0.149	$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.91	$(\Delta/\sigma)_{max} < 0.001$
3278 reflections	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
232 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.5922 (3)	0.5615 (7)	0.37528 (10)	0.0917 (11)	
H1	0.5662	0.6435	0.3572	0.110*	
C2	0.5875 (2)	0.6479 (7)	0.40946 (10)	0.0950 (12)	
H2	0.5578	0.7850	0.4140	0.114*	
C3	0.6256 (2)	0.5359 (7)	0.43673 (9)	0.0785 (10)	
C4	0.6685 (2)	0.3312 (7)	0.42919 (9)	0.0847 (11)	
H4	0.6947	0.2505	0.4473	0.102*	
C5	0.6728 (2)	0.2448 (6)	0.39472 (9)	0.0777 (10)	
H5	0.7023	0.1074	0.3901	0.093*	
C6	0.6343 (2)	0.3585 (6)	0.36719 (9)	0.0695 (9)	
C7	0.6364 (2)	0.2713 (6)	0.33017 (9)	0.0729 (9)	
H7	0.6186	0.3768	0.3128	0.087*	
C8	0.6605 (2)	0.0640 (7)	0.31933 (10)	0.0780 (10)	

H8	0.6817	−0.0376	0.3364	0.094*	
C9	0.65773 (19)	−0.0279 (7)	0.28275 (8)	0.0696 (9)	
C10	0.6515 (2)	0.1376 (5)	0.25147 (8)	0.0698 (9)	
H10A	0.6292	0.2887	0.2593	0.084*	
H10B	0.7047	0.1685	0.2423	0.084*	
C11	0.60051 (19)	0.0390 (6)	0.22233 (7)	0.0639 (8)	
H11	0.6193	−0.1239	0.2177	0.077*	
C12	0.60787 (18)	0.1753 (5)	0.18788 (7)	0.0584 (8)	
C13	0.6599 (2)	0.0985 (6)	0.16217 (9)	0.0763 (10)	
H13	0.6914	−0.0353	0.1665	0.092*	
C14	0.6667 (2)	0.2145 (7)	0.13016 (9)	0.0807 (10)	
H14	0.7020	0.1562	0.1132	0.097*	
C15	0.6221 (2)	0.4150 (6)	0.12276 (8)	0.0647 (8)	
C16	0.57100 (19)	0.4968 (6)	0.14881 (9)	0.0748 (9)	
H16	0.5404	0.6330	0.1448	0.090*	
C17	0.5650 (2)	0.3779 (6)	0.18074 (8)	0.0734 (9)	
H17	0.5307	0.4376	0.1980	0.088*	
C18A	0.6696 (8)	0.4526 (18)	0.50761 (19)	0.185 (6)	0.558 (10)
H18A	0.6800	0.5275	0.5300	0.278*	0.558 (10)
H18B	0.7194	0.4056	0.4969	0.278*	0.558 (10)
H18C	0.6367	0.3142	0.5111	0.278*	0.558 (10)
C18B	0.5447 (6)	0.868 (2)	0.4815 (2)	0.129 (5)	0.442 (10)
H18D	0.5360	0.9167	0.5056	0.194*	0.442 (10)
H18E	0.4962	0.8019	0.4721	0.194*	0.442 (10)
H18F	0.5604	1.0040	0.4677	0.194*	0.442 (10)
C19A	0.5590 (4)	0.7683 (11)	0.07904 (14)	0.103 (3)	0.645 (8)
H19A	0.5703	0.8896	0.0963	0.154*	0.645 (8)
H19B	0.5078	0.6982	0.0839	0.154*	0.645 (8)
H19C	0.5584	0.8382	0.0558	0.154*	0.645 (8)
C19B	0.6783 (9)	0.395 (2)	0.0529 (3)	0.142 (6)	0.355 (8)
H19D	0.7305	0.3581	0.0620	0.212*	0.355 (8)
H19E	0.6834	0.4812	0.0310	0.212*	0.355 (8)
H19F	0.6495	0.2490	0.0487	0.212*	0.355 (8)
N1	0.52006 (13)	0.0200 (4)	0.23479 (6)	0.0664 (7)	
H1A	0.4895	−0.0385	0.2175	0.080*	
H1B	0.5026	0.1648	0.2408	0.080*	
O1	0.66252 (17)	−0.2418 (5)	0.27820 (6)	0.0981 (8)	
S1	0.62088 (8)	0.6514 (2)	0.48013 (3)	0.1207 (5)	
S2	0.63084 (7)	0.5537 (2)	0.08090 (2)	0.0983 (4)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.125 (3)	0.075 (3)	0.075 (3)	0.013 (2)	−0.012 (2)	0.004 (2)
C2	0.125 (3)	0.083 (3)	0.077 (3)	0.018 (2)	−0.002 (2)	−0.009 (2)
C3	0.094 (3)	0.082 (2)	0.059 (2)	−0.001 (2)	0.0011 (19)	0.003 (2)
C4	0.092 (3)	0.100 (3)	0.062 (2)	0.006 (2)	−0.0071 (19)	0.018 (2)
C5	0.083 (2)	0.077 (2)	0.073 (2)	0.0083 (19)	0.005 (2)	0.002 (2)

C6	0.079 (2)	0.073 (2)	0.057 (2)	−0.009 (2)	−0.0037 (18)	0.0082 (18)
C7	0.080 (2)	0.065 (2)	0.074 (2)	−0.0024 (19)	−0.0078 (19)	0.0111 (19)
C8	0.084 (2)	0.073 (2)	0.077 (3)	−0.001 (2)	−0.0053 (19)	0.016 (2)
C9	0.077 (2)	0.071 (2)	0.061 (2)	−0.002 (2)	0.0003 (16)	0.0004 (19)
C10	0.082 (2)	0.066 (2)	0.062 (2)	−0.0021 (18)	−0.0050 (17)	0.0043 (17)
C11	0.072 (2)	0.068 (2)	0.0519 (18)	−0.0042 (17)	0.0032 (16)	−0.0025 (15)
C12	0.0608 (19)	0.062 (2)	0.0520 (18)	−0.0067 (17)	0.0006 (16)	−0.0058 (16)
C13	0.079 (2)	0.084 (2)	0.065 (2)	0.0177 (19)	0.0108 (18)	0.0042 (19)
C14	0.080 (2)	0.099 (3)	0.063 (2)	0.013 (2)	0.0220 (18)	0.000 (2)
C15	0.068 (2)	0.078 (2)	0.0483 (18)	−0.0090 (19)	0.0000 (16)	0.0006 (16)
C16	0.078 (2)	0.076 (2)	0.070 (2)	0.0085 (18)	0.0070 (19)	0.004 (2)
C17	0.086 (2)	0.080 (2)	0.0547 (19)	0.007 (2)	0.0187 (18)	−0.0008 (18)
C18A	0.335 (16)	0.165 (9)	0.055 (5)	0.048 (10)	−0.013 (7)	−0.006 (5)
C18B	0.140 (10)	0.155 (10)	0.092 (7)	0.039 (8)	−0.010 (6)	−0.011 (7)
C19A	0.102 (5)	0.126 (5)	0.080 (4)	0.002 (4)	−0.005 (3)	0.024 (4)
C19B	0.205 (14)	0.172 (13)	0.048 (7)	0.017 (11)	0.033 (8)	0.020 (7)
N1	0.0436 (14)	0.101 (2)	0.0549 (14)	−0.0148 (13)	0.0039 (11)	0.0137 (15)
O1	0.140 (2)	0.0674 (16)	0.0873 (18)	0.0104 (16)	−0.0053 (15)	0.0060 (14)
S1	0.1498 (11)	0.1446 (11)	0.0678 (7)	0.0149 (9)	0.0039 (7)	−0.0160 (7)
S2	0.1033 (8)	0.1321 (10)	0.0594 (6)	−0.0058 (7)	0.0019 (5)	0.0185 (6)

Geometric parameters (Å, °)

C1—C6	1.370 (4)	C13—H13	0.9300
C1—C2	1.379 (5)	C14—C15	1.375 (4)
C1—H1	0.9300	C14—H14	0.9300
C2—C3	1.362 (5)	C15—C16	1.379 (4)
C2—H2	0.9300	C15—S2	1.766 (3)
C3—C4	1.381 (5)	C16—C17	1.380 (4)
C3—S1	1.762 (3)	C16—H16	0.9300
C4—C5	1.389 (4)	C17—H17	0.9300
C4—H4	0.9300	C18A—S1	1.725 (9)
C5—C6	1.378 (4)	C18A—H18A	0.9600
C5—H5	0.9300	C18A—H18B	0.9600
C6—C7	1.480 (4)	C18A—H18C	0.9600
C7—C8	1.294 (4)	C18B—S1	1.758 (10)
C7—H7	0.9300	C18B—H18D	0.9600
C8—C9	1.473 (5)	C18B—H18E	0.9600
C8—H8	0.9300	C18B—H18F	0.9600
C9—O1	1.212 (4)	C19A—S2	1.699 (6)
C9—C10	1.504 (4)	C19A—H19A	0.9600
C10—C11	1.496 (4)	C19A—H19B	0.9600
C10—H10A	0.9700	C19A—H19C	0.9600
C10—H10B	0.9700	C19B—S2	1.594 (12)
C11—N1	1.428 (4)	C19B—H19D	0.9600
C11—C12	1.512 (4)	C19B—H19E	0.9600
C11—H11	0.9800	C19B—H19F	0.9600
C12—C17	1.367 (4)	N1—H1A	0.8900
C12—C13	1.372 (4)	N1—H1B	0.8900

C13—C14	1.376 (4)		
C6—C1—C2	121.9 (4)	C15—C14—C13	121.2 (3)
C6—C1—H1	119.0	C15—C14—H14	119.4
C2—C1—H1	119.0	C13—C14—H14	119.4
C3—C2—C1	121.2 (4)	C14—C15—C16	117.5 (3)
C3—C2—H2	119.4	C14—C15—S2	119.7 (3)
C1—C2—H2	119.4	C16—C15—S2	122.8 (3)
C2—C3—C4	117.9 (3)	C15—C16—C17	120.4 (3)
C2—C3—S1	120.8 (3)	C15—C16—H16	119.8
C4—C3—S1	121.3 (3)	C17—C16—H16	119.8
C3—C4—C5	120.6 (3)	C12—C17—C16	122.3 (3)
C3—C4—H4	119.7	C12—C17—H17	118.9
C5—C4—H4	119.7	C16—C17—H17	118.9
C6—C5—C4	121.4 (3)	S1—C18A—H18A	109.5
C6—C5—H5	119.3	S1—C18A—H18B	109.5
C4—C5—H5	119.3	H18A—C18A—H18B	109.5
C1—C6—C5	117.0 (3)	S1—C18A—H18C	109.5
C1—C6—C7	119.8 (3)	H18A—C18A—H18C	109.5
C5—C6—C7	123.2 (3)	H18B—C18A—H18C	109.5
C8—C7—C6	127.0 (3)	S1—C18B—H18D	109.5
C8—C7—H7	116.5	S1—C18B—H18E	109.5
C6—C7—H7	116.5	H18D—C18B—H18E	109.5
C7—C8—C9	126.8 (3)	S1—C18B—H18F	109.5
C7—C8—H8	116.6	H18D—C18B—H18F	109.5
C9—C8—H8	116.6	H18E—C18B—H18F	109.5
O1—C9—C8	118.4 (3)	S2—C19A—H19A	109.5
O1—C9—C10	120.1 (3)	S2—C19A—H19B	109.5
C8—C9—C10	121.5 (3)	H19A—C19A—H19B	109.5
C11—C10—C9	112.9 (3)	S2—C19A—H19C	109.5
C11—C10—H10A	109.0	H19A—C19A—H19C	109.5
C9—C10—H10A	109.0	H19B—C19A—H19C	109.5
C11—C10—H10B	109.0	S2—C19B—H19D	109.5
C9—C10—H10B	109.0	S2—C19B—H19E	109.5
H10A—C10—H10B	107.8	H19D—C19B—H19E	109.5
N1—C11—C10	108.7 (2)	S2—C19B—H19F	109.5
N1—C11—C12	113.4 (3)	H19D—C19B—H19F	109.5
C10—C11—C12	113.5 (3)	H19E—C19B—H19F	109.5
N1—C11—H11	106.9	C11—N1—H1A	109.0
C10—C11—H11	106.9	C11—N1—H1B	108.9
C12—C11—H11	106.9	H1A—N1—H1B	109.5
C17—C12—C13	116.9 (3)	C18A—S1—C18B	140.2 (5)
C17—C12—C11	123.0 (3)	C18A—S1—C3	107.5 (3)
C13—C12—C11	120.1 (3)	C18B—S1—C3	108.2 (3)
C12—C13—C14	121.7 (3)	C19B—S2—C19A	135.9 (5)
C12—C13—H13	119.2	C19B—S2—C15	112.9 (5)
C14—C13—H13	119.2	C19A—S2—C15	106.8 (2)
C6—C1—C2—C3	0.9 (6)	N1—C11—C12—C13	−139.8 (3)
C1—C2—C3—C4	−0.7 (6)	C10—C11—C12—C13	95.4 (4)

C1—C2—C3—S1	178.6 (3)	C17—C12—C13—C14	−2.3 (5)
C2—C3—C4—C5	0.5 (5)	C11—C12—C13—C14	178.3 (3)
S1—C3—C4—C5	−178.8 (3)	C12—C13—C14—C15	0.9 (5)
C3—C4—C5—C6	−0.5 (5)	C13—C14—C15—C16	0.7 (5)
C2—C1—C6—C5	−0.9 (5)	C13—C14—C15—S2	−178.4 (3)
C2—C1—C6—C7	179.0 (4)	C14—C15—C16—C17	−0.7 (5)
C4—C5—C6—C1	0.6 (5)	S2—C15—C16—C17	178.4 (3)
C4—C5—C6—C7	−179.3 (3)	C13—C12—C17—C16	2.3 (5)
C1—C6—C7—C8	−166.6 (4)	C11—C12—C17—C16	−178.3 (3)
C5—C6—C7—C8	13.3 (5)	C15—C16—C17—C12	−0.8 (5)
C6—C7—C8—C9	175.8 (3)	C2—C3—S1—C18A	175.8 (5)
C7—C8—C9—O1	−161.0 (4)	C4—C3—S1—C18A	−4.9 (6)
C7—C8—C9—C10	20.7 (5)	C2—C3—S1—C18B	13.6 (5)
O1—C9—C10—C11	38.2 (4)	C4—C3—S1—C18B	−167.1 (5)
C8—C9—C10—C11	−143.5 (3)	C14—C15—S2—C19B	11.9 (7)
C9—C10—C11—N1	65.4 (3)	C16—C15—S2—C19B	−167.2 (7)
C9—C10—C11—C12	−167.4 (3)	C14—C15—S2—C19A	172.4 (3)
N1—C11—C12—C17	40.8 (4)	C16—C15—S2—C19A	−6.7 (4)
C10—C11—C12—C17	−84.0 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1B···N1^{i}	0.89	2.22	3.0981 (19)	167

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2.

Fig. 1

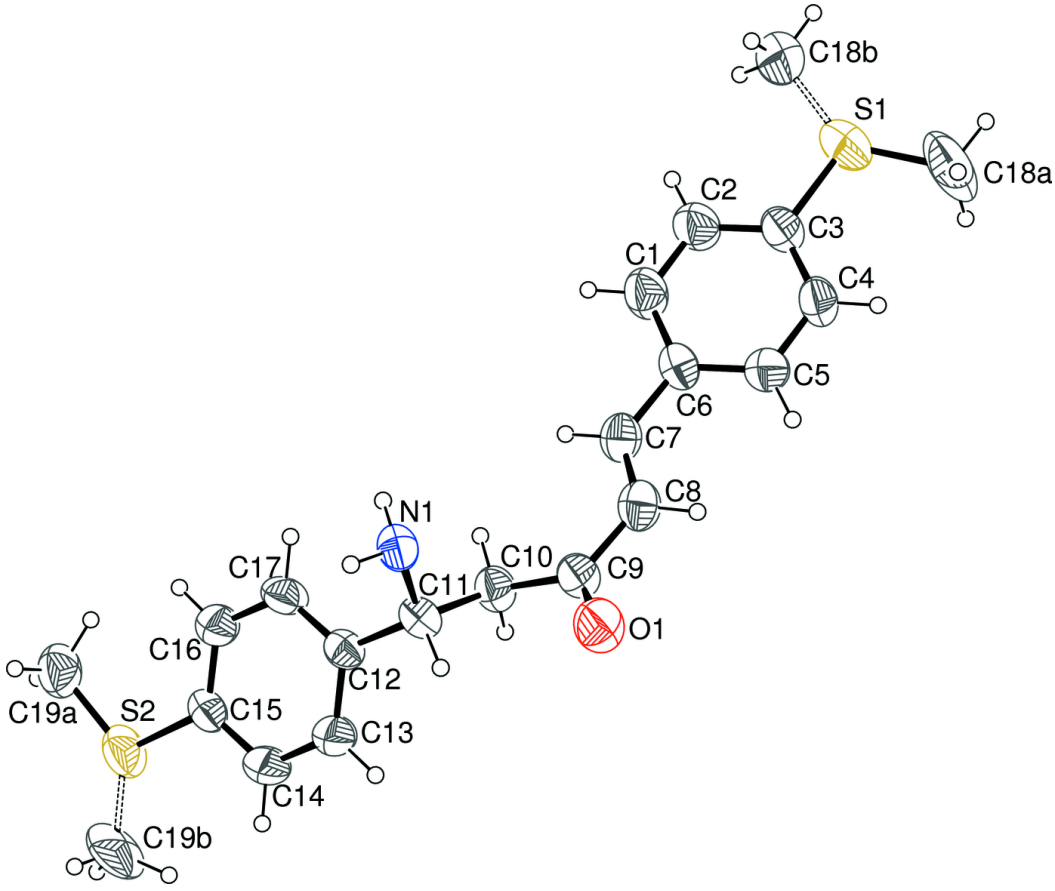
C18b
S1
C18a
C2
C3
C1
C4
C5
C6
C7
C8
N1
C10
C9
C17
C11
O1
C16
C12
C19a
S2
C15
C13
C14
C19b

Fig. 2