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N-(3,4-Dichlorophenyl)-*N*′-decanoylthiourea

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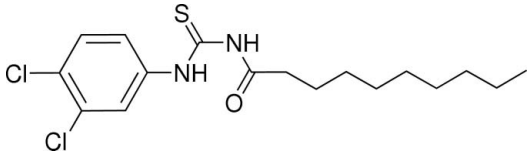
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.045; wR factor = 0.115; data-to-parameter ratio = 18.1.

The title compound, $C_{17}H_{24}Cl_2N_2OS$, adopts a *trans–cis* configuration of the decanoyl and 3,4-dichlorophenyl groups with respect to the thiono S atom across the thiourea C—N bonds. The crystal structure is stabilized by intermolecular N—H···S and C—H···S hydrogen bonds, forming dimers parallel to the *b* axis.

Related literature

For related crystal structures, see: Yusof, Ramlee *et al.* (2007); Yusof, Yaakob *et al.* (2007). For details of potential applications in materials and biological activities, see: Wei *et al.* (2004); Baruah *et al.* (2002). For related literature, see: Allen *et al.* (1987); Yusof *et al.* (2006).



Experimental

Crystal data

$C_{17}H_{24}Cl_2N_2OS$
M_r = 375.34
Triclinic, $P\overline{1}$
a = 4.7368 (13) Å
b = 11.295 (3) Å
c = 18.324 (5) Å
α = 88.289 (5)°
β = 83.774 (5)°
γ = 84.268 (4)°
V = 969.5 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 293 (2) K
0.46 × 0.41 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.821, T_{max} = 0.961
10011 measured reflections
3778 independent reflections
2856 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.115
S = 1.04
3778 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1	0.86	1.90	2.627 (2)	142
C17—H17···S1	0.93	2.54	3.207 (3)	129
N1—H1···S1^{i}	0.86	2.62	3.461 (2)	166
C9—H9*A*···S1^{i}	0.97	2.84	3.552 (3)	131

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2267).

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supplementary materials

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N-(3,4-Dichlorophenyl)-*N*'-decanoylthiourea

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Comment

Thiourea derivatives receive considerable attention because of their potential applications in materials science (Wei *et al.*, 2004) and their biological activities (Baruah *et al.*, 2002). The title compound, (I), is similar to *N*-(3,4-Dichlorophenyl)-*N*'-(3-nitrobenzoyl)thiourea, (Yusof *et al.*, 2006), except that the 3-nitrobenzoyl group is replaced by a decanoyl group (Fig.1). The molecule maintains its *trans-cis* configuration with respect to the position of the decanoyl and 3,4-dichlorophenyl groups relative to the thiono S1 atom across their C—N bonds, respectively. The bond lengths and angles are in normal ranges (Allen *et al.*, 1987) and comparable with other thiourea derivatives (Yusof, Ramlee *et al.* (2007); Yusof, Yaakob *et al.* (2007). The thiourea-3,4-dichlorophenyl (S1/N1/N2/C11—C17/Cl1/Cl2) fragment are essentially planar with a maximum deviation of 0.039 (2)Å for atom C10 from the least-squares plane.

There are two intramolecular hydrogen bonds, N2—H2···O1 and C17—H17···S1 (Table 2), forming two pseudo-six-membered rings (O1···H2—N2—C11—N1—C10—O1 and S1···H17—C17—C12—N2—C11—S1). In the crystal structure, the molecules are linked by intermolecular interactions, N—H···S and C—H···S (symmetry codes as in Table 2) forming dimers parallel to *b* axis (Fig.2).

Experimental

To a stirring acetone solution (75 ml) of decanoyl chloride (2.0 g, 10 mmol) and ammoniumthiocyanate (0.80 g, 10 mmol), 3,4-dichloroaniline (1.70 g, 10 mmol) in 40 ml of acetone was added dropwise. The solution mixture was refluxed for 1 h. The resulting solution was poured into a beaker containing some ice blocks. The white precipitate was filtered off and washed with distilled water and cold ethanol before dried under vacuum. Good quality crystals were obtained by recrystallization from THF. Yield 75% (2.31 g).

Refinement

After their location in the difference map, all H-atoms were fixed geometrically at ideal positions and allowed to ride on the parent C or N atoms with C—H = 0.93–0.97Å and N—H = 0.86Å with U_{iso}(H)= 1.2 (CH_2 and NH) or 1.5U_{eq}(C)(CH_3).

Figures

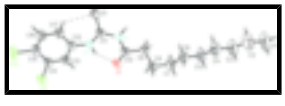

Fig. 1. : The molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate hydrogen bonds.

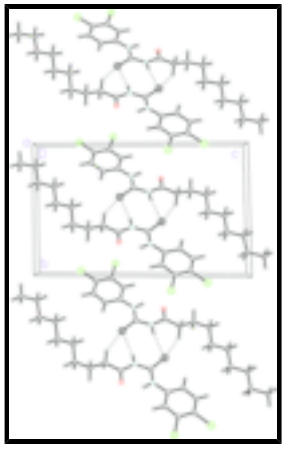

Fig. 2. : Packing diagram of compound,(I), viewed down the *b* axis. The dashed lines denote the N—H···S and C—H···S hydrogen bonds.

N-(3,4-Dichlorophenyl)-*N*'-decanoylthiourea

Crystal data

$C_{17}H_{24}Cl_2N_2OS$	$Z = 2$
$M_r = 375.34$	$F_{000} = 396$
Triclinic, $P\overline{1}$	$D_x = 1.286$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 4.7368$ (13) Å	Cell parameters from 797 reflections
$b = 11.295$ (3) Å	$\theta = 1.8$–25.9º
$c = 18.324$ (5) Å	$\mu = 0.45$ mm^{-1}
$\alpha = 88.289$ (5)º	$T = 293$ (2) K
$\beta = 83.774$ (5)º	Slab, colourless
$\gamma = 84.268$ (4)º	0.46 × 0.41 × 0.09 mm
$V = 969.5$ (5) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3778 independent reflections
Radiation source: fine-focus sealed tube	2856 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.027$
Detector resolution: 83.66 pixels mm^{-1}	$\theta_{max} = 26.0$º
$T = 293(2)$ K	$\theta_{min} = 1.8$º
ω scans	$h = -5 \rightarrow 5$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$k = -13 \rightarrow 13$
$T_{min} = 0.821$, $T_{max} = 0.961$	$l = -22 \rightarrow 22$
10011 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.115$	$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 0.1967P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
3778 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
209 parameters	$\Delta\rho_{min} = -0.14$ 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 $F^2 > 2$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}
Cl1	0.01781 (13)	−0.07409 (5)	0.37362 (4)	0.0680 (2)
Cl2	0.2794 (2)	−0.02429 (7)	0.21084 (4)	0.0968 (3)
S1	0.91305 (13)	0.40736 (5)	0.40393 (3)	0.05798 (19)
O1	0.3719 (3)	0.26352 (14)	0.59943 (8)	0.0627 (4)
N1	0.7140 (4)	0.36909 (14)	0.54034 (9)	0.0481 (4)
H1	0.8297	0.4205	0.5476	0.058*
N2	0.5577 (4)	0.24761 (15)	0.45933 (10)	0.0517 (4)
H2	0.4722	0.2223	0.4998	0.062*
C1	0.9528 (12)	0.8466 (4)	1.0584 (2)	0.1484 (18)
H1A	0.8029	0.8256	1.0945	0.223*
H1B	0.9753	0.9298	1.0616	0.223*
H1C	1.1280	0.8006	1.0670	0.223*
C2	0.8783 (11)	0.8216 (3)	0.9835 (2)	0.1307 (15)
H2A	0.7070	0.8720	0.9745	0.157*
H2B	1.0311	0.8436	0.9476	0.157*
C3	0.8308 (9)	0.6977 (3)	0.97181 (18)	0.1074 (11)
H3A	0.6837	0.6750	1.0091	0.129*
H3B	1.0048	0.6479	0.9792	0.129*
C4	0.7440 (8)	0.6707 (3)	0.89723 (16)	0.0951 (9)
H4A	0.5734	0.7221	0.8889	0.114*
H4B	0.8942	0.6900	0.8598	0.114*
C5	0.6872 (7)	0.5449 (3)	0.88831 (15)	0.0873 (9)

H5A	0.5416	0.5250	0.9269	0.105*
H5B	0.8598	0.4939	0.8954	0.105*
C6	0.5922 (6)	0.5167 (2)	0.81562 (13)	0.0747 (7)
H6A	0.4186	0.5668	0.8084	0.090*
H6B	0.7373	0.5360	0.7768	0.090*
C7	0.5383 (7)	0.3888 (3)	0.80900 (14)	0.0787 (8)
H7A	0.4022	0.3685	0.8498	0.094*
H7B	0.7152	0.3394	0.8137	0.094*
C8	0.4263 (5)	0.3578 (2)	0.73827 (13)	0.0658 (6)
H8A	0.3892	0.2748	0.7406	0.079*
H8B	0.2470	0.4055	0.7335	0.079*
C9	0.6313 (5)	0.3787 (2)	0.67181 (12)	0.0550 (6)
H9A	0.6436	0.4637	0.6655	0.066*
H9B	0.8189	0.3422	0.6807	0.066*
C10	0.5548 (4)	0.33149 (18)	0.60210 (12)	0.0502 (5)
C11	0.7161 (4)	0.33642 (17)	0.46781 (11)	0.0448 (5)
C12	0.5032 (4)	0.18709 (18)	0.39686 (12)	0.0478 (5)
C13	0.3189 (4)	0.09942 (18)	0.41067 (12)	0.0499 (5)
H13	0.2411	0.0848	0.4585	0.060*
C14	0.2497 (4)	0.03368 (18)	0.35420 (13)	0.0515 (5)
C15	0.3639 (5)	0.0554 (2)	0.28369 (13)	0.0600 (6)
C16	0.5490 (6)	0.1417 (2)	0.26975 (14)	0.0665 (7)
H16	0.6266	0.1557	0.2218	0.080*
C17	0.6212 (5)	0.2079 (2)	0.32576 (13)	0.0613 (6)
H17	0.7476	0.2657	0.3159	0.074*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0635 (4)	0.0518 (3)	0.0937 (5)	−0.0211 (3)	−0.0138 (3)	−0.0129 (3)
Cl2	0.1279 (7)	0.0942 (5)	0.0775 (5)	−0.0338 (5)	−0.0231 (4)	−0.0307 (4)
S1	0.0643 (4)	0.0517 (3)	0.0606 (4)	−0.0245 (3)	−0.0003 (3)	−0.0033 (3)
O1	0.0618 (10)	0.0693 (10)	0.0627 (10)	−0.0372 (8)	−0.0035 (8)	−0.0062 (8)
N1	0.0472 (10)	0.0453 (9)	0.0553 (11)	−0.0194 (8)	−0.0065 (8)	−0.0065 (8)
N2	0.0549 (11)	0.0517 (10)	0.0523 (10)	−0.0232 (9)	−0.0059 (8)	−0.0036 (8)
C1	0.246 (5)	0.117 (3)	0.099 (3)	−0.070 (3)	−0.043 (3)	−0.014 (2)
C2	0.205 (5)	0.100 (3)	0.100 (3)	−0.049 (3)	−0.042 (3)	−0.010 (2)
C3	0.158 (3)	0.092 (2)	0.081 (2)	−0.035 (2)	−0.033 (2)	−0.0059 (17)
C4	0.134 (3)	0.089 (2)	0.0673 (18)	−0.0217 (19)	−0.0211 (18)	−0.0084 (15)
C5	0.118 (2)	0.091 (2)	0.0575 (16)	−0.0275 (18)	−0.0122 (16)	−0.0076 (14)
C6	0.096 (2)	0.0782 (18)	0.0521 (14)	−0.0202 (15)	−0.0076 (13)	−0.0066 (12)
C7	0.098 (2)	0.089 (2)	0.0534 (15)	−0.0347 (16)	−0.0063 (14)	0.0052 (13)
C8	0.0718 (16)	0.0731 (16)	0.0562 (14)	−0.0297 (13)	−0.0043 (12)	0.0029 (12)
C9	0.0527 (13)	0.0580 (13)	0.0576 (13)	−0.0179 (10)	−0.0080 (10)	−0.0038 (10)
C10	0.0464 (12)	0.0463 (12)	0.0600 (14)	−0.0113 (10)	−0.0082 (10)	−0.0035 (10)
C11	0.0399 (11)	0.0372 (10)	0.0588 (13)	−0.0051 (8)	−0.0092 (9)	−0.0042 (9)
C12	0.0480 (12)	0.0434 (11)	0.0541 (13)	−0.0087 (9)	−0.0108 (10)	−0.0039 (9)
C13	0.0472 (12)	0.0451 (11)	0.0584 (13)	−0.0068 (9)	−0.0074 (10)	−0.0050 (10)

C14	0.0479 (12)	0.0414 (11)	0.0682 (15)	−0.0083 (9)	−0.0140 (11)	−0.0081 (10)
C15	0.0673 (15)	0.0541 (13)	0.0625 (15)	−0.0081 (11)	−0.0190 (12)	−0.0138 (11)
C16	0.0820 (17)	0.0647 (15)	0.0558 (14)	−0.0194 (13)	−0.0082 (12)	−0.0041 (11)
C17	0.0717 (16)	0.0548 (13)	0.0608 (15)	−0.0220 (12)	−0.0080 (12)	−0.0013 (11)

Geometric parameters (Å, °)

Cl1—C14	1.724 (2)	C5—H5A	0.9700
Cl2—C15	1.736 (2)	C5—H5B	0.9700
S1—C11	1.655 (2)	C6—C7	1.503 (4)
O1—C10	1.219 (2)	C6—H6A	0.9700
N1—C10	1.371 (3)	C6—H6B	0.9700
N1—C11	1.389 (3)	C7—C8	1.515 (3)
N1—H1	0.8600	C7—H7A	0.9700
N2—C11	1.333 (2)	C7—H7B	0.9700
N2—C12	1.411 (2)	C8—C9	1.501 (3)
N2—H2	0.8600	C8—H8A	0.9700
C1—C2	1.495 (4)	C8—H8B	0.9700
C1—H1A	0.9600	C9—C10	1.492 (3)
C1—H1B	0.9600	C9—H9A	0.9700
C1—H1C	0.9600	C9—H9B	0.9700
C2—C3	1.465 (4)	C12—C17	1.384 (3)
C2—H2A	0.9700	C12—C13	1.384 (3)
C2—H2B	0.9700	C13—C14	1.378 (3)
C3—C4	1.517 (4)	C13—H13	0.9300
C3—H3A	0.9700	C14—C15	1.370 (3)
C3—H3B	0.9700	C15—C16	1.375 (3)
C4—C5	1.489 (4)	C16—C17	1.379 (3)
C4—H4A	0.9700	C16—H16	0.9300
C4—H4B	0.9700	C17—H17	0.9300
C5—C6	1.504 (3)		
C10—N1—C11	129.58 (17)	C6—C7—C8	115.6 (2)
C10—N1—H1	115.2	C6—C7—H7A	108.4
C11—N1—H1	115.2	C8—C7—H7A	108.4
C11—N2—C12	132.43 (18)	C6—C7—H7B	108.4
C11—N2—H2	113.8	C8—C7—H7B	108.4
C12—N2—H2	113.8	H7A—C7—H7B	107.4
C2—C1—H1A	109.5	C9—C8—C7	112.5 (2)
C2—C1—H1B	109.5	C9—C8—H8A	109.1
H1A—C1—H1B	109.5	C7—C8—H8A	109.1
C2—C1—H1C	109.5	C9—C8—H8B	109.1
H1A—C1—H1C	109.5	C7—C8—H8B	109.1
H1B—C1—H1C	109.5	H8A—C8—H8B	107.8
C3—C2—C1	115.0 (3)	C10—C9—C8	114.85 (18)
C3—C2—H2A	108.5	C10—C9—H9A	108.6
C1—C2—H2A	108.5	C8—C9—H9A	108.6
C3—C2—H2B	108.5	C10—C9—H9B	108.6
C1—C2—H2B	108.5	C8—C9—H9B	108.6
H2A—C2—H2B	107.5	H9A—C9—H9B	107.5

C2—C3—C4	116.1 (3)	O1—C10—N1	122.20 (19)
C2—C3—H3A	108.3	O1—C10—C9	123.8 (2)
C4—C3—H3A	108.3	N1—C10—C9	114.00 (17)
C2—C3—H3B	108.3	N2—C11—N1	113.74 (18)
C4—C3—H3B	108.3	N2—C11—S1	128.19 (16)
H3A—C3—H3B	107.4	N1—C11—S1	118.06 (14)
C5—C4—C3	114.6 (3)	C17—C12—C13	119.6 (2)
C5—C4—H4A	108.6	C17—C12—N2	125.30 (19)
C3—C4—H4A	108.6	C13—C12—N2	115.07 (18)
C5—C4—H4B	108.6	C14—C13—C12	120.6 (2)
C3—C4—H4B	108.6	C14—C13—H13	119.7
H4A—C4—H4B	107.6	C12—C13—H13	119.7
C4—C5—C6	115.6 (2)	C15—C14—C13	119.7 (2)
C4—C5—H5A	108.4	C15—C14—Cl1	121.13 (17)
C6—C5—H5A	108.4	C13—C14—Cl1	119.17 (18)
C4—C5—H5B	108.4	C14—C15—C16	119.9 (2)
C6—C5—H5B	108.4	C14—C15—Cl2	121.17 (18)
H5A—C5—H5B	107.4	C16—C15—Cl2	118.9 (2)
C7—C6—C5	113.8 (2)	C15—C16—C17	121.0 (2)
C7—C6—H6A	108.8	C15—C16—H16	119.5
C5—C6—H6A	108.8	C17—C16—H16	119.5
C7—C6—H6B	108.8	C16—C17—C12	119.1 (2)
C5—C6—H6B	108.8	C16—C17—H17	120.4
H6A—C6—H6B	107.7	C12—C17—H17	120.4
C1—C2—C3—C4	177.8 (4)	C11—N2—C12—C17	2.1 (4)
C2—C3—C4—C5	−177.9 (4)	C11—N2—C12—C13	−178.9 (2)
C3—C4—C5—C6	178.2 (3)	C17—C12—C13—C14	−0.7 (3)
C4—C5—C6—C7	179.8 (3)	N2—C12—C13—C14	−179.76 (17)
C5—C6—C7—C8	176.7 (3)	C12—C13—C14—C15	−0.1 (3)
C6—C7—C8—C9	61.8 (3)	C12—C13—C14—Cl1	−179.65 (17)
C7—C8—C9—C10	170.5 (2)	C13—C14—C15—C16	0.7 (3)
C11—N1—C10—O1	−3.9 (3)	Cl1—C14—C15—C16	−179.83 (19)
C11—N1—C10—C9	174.66 (19)	C13—C14—C15—Cl2	−179.33 (16)
C8—C9—C10—O1	−12.4 (3)	Cl1—C14—C15—Cl2	0.2 (3)
C8—C9—C10—N1	169.1 (2)	C14—C15—C16—C17	−0.4 (4)
C12—N2—C11—N1	−179.19 (19)	Cl2—C15—C16—C17	179.6 (2)
C12—N2—C11—S1	−0.6 (3)	C15—C16—C17—C12	−0.4 (4)
C10—N1—C11—N2	−6.8 (3)	C13—C12—C17—C16	1.0 (3)
C10—N1—C11—S1	174.47 (17)	N2—C12—C17—C16	179.9 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	0.86	1.90	2.627 (2)	142
C17—H17···S1	0.93	2.54	3.207 (3)	129
N1—H1···S1^{i}	0.86	2.62	3.461 (2)	166
C9—H9A···S1^{i}	0.97	2.84	3.552 (3)	131

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

Fig. 1

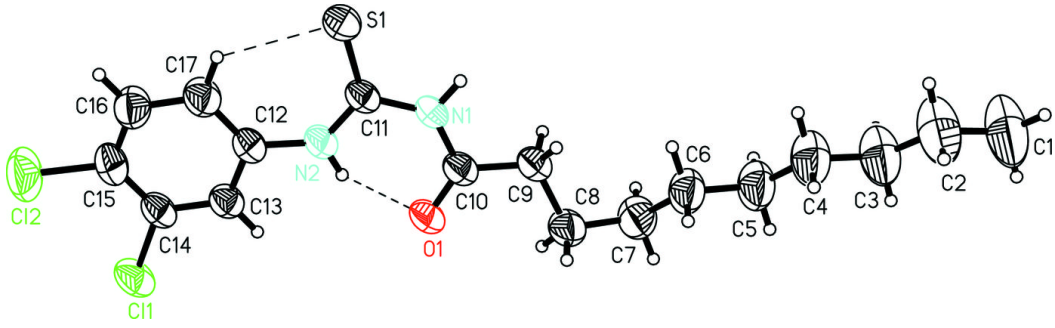
S1
C17
C16
C12
C11
N1
N2
C10
C9
C8
C6
C5
C4
C3
C2
C1
C15
C13
Cl2
C14
O1
C7
Cl1

Fig. 2