Cl1*B*	0.6749 (2)	0.07701 (14)	0.95369 (6)	0.0738 (5)
Cl2*B*	0.82194 (14)	−0.22292 (11)	0.97865 (5)	0.0513 (3)
S1*B*	0.98095 (10)	−0.00257 (8)	0.80560 (5)	0.0315 (2)
N1*B*	0.7120 (3)	0.0188 (3)	0.8319 (2)	0.0304 (8)
N2*B*	0.8133 (4)	−0.1454 (3)	0.86052 (15)	0.0300 (8)
C1*B*	0.8278 (4)	−0.0460 (3)	0.8347 (2)	0.0262 (8)
C2*B*	0.5772 (4)	−0.0061 (3)	0.8558 (2)	0.0286 (9)
C3*B*	0.4718 (4)	−0.0506 (3)	0.8232 (2)	0.0311 (9)
C4*B*	0.3381 (5)	−0.0695 (4)	0.8454 (2)	0.0420 (12)
C5*B*	0.3090 (5)	−0.0447 (4)	0.8998 (2)	0.0465 (12)
C6*B*	0.4133 (6)	−0.0016 (5)	0.9325 (2)	0.0496 (13)
C7*B*	0.5477 (5)	0.0203 (4)	0.9115 (2)	0.0387 (11)
C8*B*	0.9220 (4)	−0.2248 (3)	0.8722 (2)	0.0266 (8)
C9*B*	1.0098 (4)	−0.2657 (3)	0.8304 (2)	0.0304 (9)
C10*B*	1.1133 (5)	−0.3449 (3)	0.8431 (2)	0.0362 (11)
C11*B*	1.1255 (5)	−0.3852 (4)	0.8970 (2)	0.0400 (12)
C12*B*	1.0375 (5)	−0.3485 (4)	0.9384 (2)	0.0379 (10)
C13*B*	0.9345 (4)	−0.2676 (4)	0.9259 (2)	0.0315 (9)

Table 2. *Comparison of selected geometry (Å, °) of the two molecules of OCDPTU*

	Molecule *A*	Molecule *B*
Cl1—C7	1.724 (4)	1.710 (5)
Cl2—C13	1.728 (5)	1.734 (4)
S1—C1	1.682 (4)	1.687 (4)
N1—C1	1.351 (5)	1.342 (5)
N1—C2	1.428 (5)	1.428 (5)
N2—C1	1.339 (5)	1.343 (5)
N2—C8	1.433 (5)	1.424 (5)
C1—N1—C2	126.7 (3)	126.0 (3)
C1—N2—C8	122.8 (3)	127.0 (3)
N2—C1—N1	117.4 (3)	116.6 (4)
N2—C1—S1	121.9 (3)	120.1 (3)
N1—C1—S1	120.7 (3)	123.2 (3)
C3—C2—N1	121.1 (4)	120.0 (4)
C7—C2—N1	119.9 (4)	120.9 (4)
C2—C7—Cl1	119.8 (3)	120.8 (3)
C13—C8—N2	120.7 (4)	121.6 (4)
C9—C8—N2	119.6 (4)	119.1 (4)
C8—C13—Cl2	119.8 (3)	120.6 (3)
C12—C13—Cl2	119.6 (4)	118.8 (3)
C2—N1—C1—S1	−176.1 (3)	−178.3 (3)
C8—N2—C1—S1	5.7 (6)	5.8 (5)
C1—N1—C2—C3	−83.1 (5)	−98.6 (5)
C1—N2—C8—C9	−88.3 (5)	−54.1 (6)

The intensity data for the title compound were collected at 173 K using a Siemens LT-2 attachment since there was large peak broadening at room temperature. The structure was solved by direct methods and refined by the full-matrix least-squares technique. All the H atoms were located from difference maps and refined isotropically. *PARST* (Nardelli, 1983) was used for geometric calculations.

Data collection: *XSCANS* (Siemens, 1994). Cell refinement: *XSCANS*. Data reduction: *XSCANS*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990*a*). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC* (Sheldrick, 1990*b*). Software used to prepare material for publication: *SHELXL*93.

One of the authors (KS) thanks the Universiti Sains Malaysia for a Visiting Post Doctoral Research Fellowship.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AS1197). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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N-[3-Methyl-2(3*H*)-thiazolylidene]benzamide Containing a Short Intramolecular S···O Contact

David P. Hansell,[a]* Kathryn J. Robinson,[a] John D. Wallis[a] and David C. Povey[b]

[a]*Chemical Laboratory, University of Kent, Canterbury CT2 7NH, England, and* [b]*Department of Chemistry, University of Surrey, Guildford GU2 5XH, England*

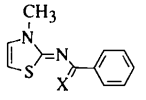
(*Received 24 July 1995; accepted 21 August 1995*)

Abstract

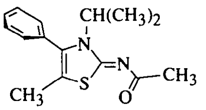
The title molecule, $C_{11}H_{10}N_2OS$, shows a short intramolecular S···O contact of 2.622 (1) Å, *ca* 0.6 Å less than the sum of the traditional van der Waals radii. Electrostatic attraction, due to charge delocalization from the heterocycle into the carbonyl group, contributes to this short interaction.

Comment

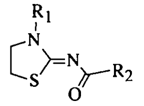
The van der Waals radii of atoms (Bondi, 1964) are not always a good guide for estimating minimum inter- and intramolecular contact distances. It is necessary to consider any effects producing attractive interactions, such as HOMO/LUMO interactions (Bürgi, Dunitz & Schefter, 1973) and cooperative interactions, and to allow for the asymmetric shape of certain bonded atoms (Nyberg & Faerman, 1985). The two latter factors contribute to the short intramolecular S···S contact in compound (1) [2.926 (1) Å; Hudson, Wallis & Hansell, 1994]. Delocalization of π-electron density from the heterocycle into the thiocarbonyl group produces a coulombic attraction between the S atoms. In addition, the effective size of the ring S atom in the plane of the heterocycle is *ca* 0.15 Å less than the traditional van der Waals radius (which corresponds more closely to the size perpendicular to the plane). This can be accounted for by the in-plane lone pair of the S atom occupying an orbital of high *s* character, in contrast to the spatially more extensive orbital of high *p* character perpendicular to the group (Hudson, Wallis & Hansell, 1994). We now report on the structure of the carbonyl analogue, (2).



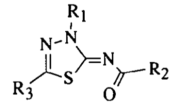
(1) X = S
(2) X = O



(3)



(4) $R_1 = H$; $R_2 = C_6H_5$
(5) $R_1 = H$; $R_2 = 2\text{-}NO_2\text{-}C_6H_4$
(6) $R_1 = H$; $R_2 = 2\text{-}Cl\text{-}C_6H_4$
(7) $R_1 = CH_3$; $R_2 = C_6H_5$



(8) $R_1 = R_2 = R_3 = C_6H_5$
(9) $R_1 = CH_3$; $R_2 = CH_3$; $R_3 = SO_2NH_2$

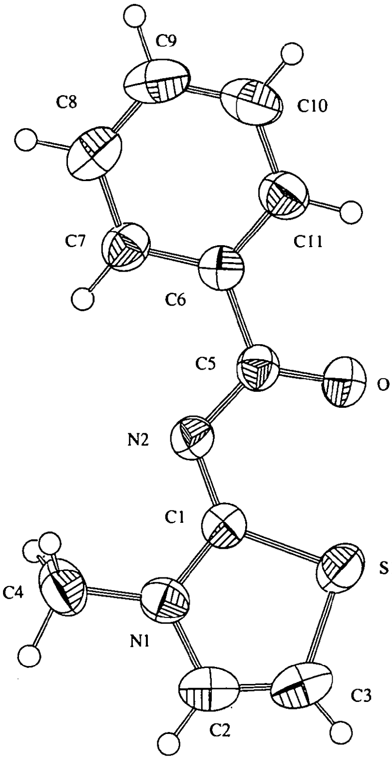


Fig. 1. The molecular structure of compound (2) (*PLUTON93*; Spek, 1993). Displacement ellipsoids are drawn at the 50% probability level.

The title molecule adopts a conformation similar to that of (1). The thiazole ring and amide group are not far from being coplanar [the interplanar angle is 7.5 (1)°] and there is a short 1,5 S···O contact of 2.622 (1) Å which is *ca* 0.6 Å less than the sum of traditional van der Waals radii. The O(1)···S(1)—C(3) angle is 162.6 (1)°. Angular distortions from idealized geometry at atoms C(1) and C(5) increase the S···O separation, suggesting that a shorter contact distance would be repulsive in this case [S(1)—C(1)—N(2) is greater than N(1)—C(1)—N(2) by 8.5° and N(2)—C(5)—O(1) is greater than O(1)—C(5)—C(6) by 5.0°]. There is structural evidence of π-electron delocalization from the heterocyclic ring into the carbonyl group leading to the development of an electrostatic S···O attraction; the three bonds N(1)—C(1), C(1)—N(2) and N(2)—C(5) are similar in length and all in the range 1.319 (2) to 1.353 (2) Å. The best plane of the phenyl group lies at 20.4 (1)° to that of the thiazole. There are no short intermolecular interactions.

There is structural data for only one directly comparable system, (3), which shows a shorter S···O contact distance [2.566 (3) Å; Declercq, De Kimpe & Boelens, 1993]. The heterocyclic ring and acetylimino substituent are exactly coplanar due to crystallographic mirror symmetry and there is structural evidence for a significantly higher degree of electron delocalization from the S atom into the carbonyl group than in compound (2). This may be due to the repulsion between the adjacent methyl and phenyl substituents on the thiazole ring, which destabilizes the π-electron structure of the heterocyclic ring (the ring C=C double bond is lengthened by *ca* 0.03 Å) and thus makes the sulfur π lone pair more available for delocalization into the exocyclic system. The 2-iminothiazolidines, compounds (4)–(7), all show slightly longer S···O contact distances than compound (2) [2.638 (4)–2.684 (2) Å, average 2.66 Å], since delocalization of electrons out of the thiazolidine ring is not promoted by a gain in aromaticity [as for (2); Cohen-Addad 1982; Cohen-Addad, Savariault & Lehmann, 1981; Kálmán & Párkányi, 1980]. The reduced degree of electron delocalization from sulfur is indicated by the increased lengths of the corresponding S(1)—C(1) bonds [1.749 (4)–1.767 (5) Å] in comparison to compound (2) [1.737 (2) Å]. [Measurement of bonding electron density in compound (6) showed no evidence for accumulation of electron density between the S and O atoms (Cohen-Addad, Savariault & Lehmann, 1981).] Nevertheless, the degree of electron delocalization is not the only factor in determining the length of the S···O contact. The 1,3,4-thiadiazole derivatives, (8) and (9), show a higher degree of double-bond localization along the S—C=N—C=O pathway when compared to compound (2), yet show shorter S···O contact distances [2.558 (6) and 2.538 (2) Å; Fukutani, Tsukihara, Okuda, Fukuyama, Katsube, Yamamoto & Gotoh, 1979; Alzuet, Ferrer, Borras & Solans, 1991]. The replacement of the 4-C atom with a more electronegative N atom acts to contract the in-plane lone pair of the S atom slightly and thus reduce the effective size of the atom. Alternatively, replacement of the 5-C atom with an N atom leads to significantly shorter S···O distances (*ca* 2.3 Å), since electron density of the O atom can overlap with a lobe of the S—N antibonding orbital (L'Abbé, Vermeulen, Toppet, King, Aerts & Sengier, 1981; Kaugars, Atherton & Han, 1992).

Experimental

Treatment of 2-aminothiazole with iodomethane in ethanol followed by reaction with benzoyl chloride in pyridine gave compound (2) (m.p. 386–388 K). δ_H ($CDCl_3$): 8.34 (2H, *m*, 2′-H, 6′-H), 7.44 (3H, *m*, 3′-H, 4′-H, 5′-H), 6.89 (1H, J = 4.7 Hz, 4-H), 6.56 (1H, J = 4.7 Hz, 5-H), 3.73 (3H, *s*, CH_3); δ_C ($CDCl_3$): 173.7 (C═O), 167.7 (2-C), 137.0 (1′-C), 131.4 (4′-C), 129.1 (2′-C, 6′-C), 128.0 (3′-C, 4′-C), 126.9 (4-C) 108.7 (5-C), 35.6 (CH_3); ν_{max}: 1596, 1546, 1406, 1108, 1066, 1026, 976, 870, 712, 684, 630 cm^{-1}.

Crystal data

$C_{11}H_{10}N_2OS$
$M_r = 218.27$
Orthorhombic
Pbca
$a = 8.446 (3)$ Å
$b = 23.758 (8)$ Å
$c = 10.454 (2)$ Å
$V = 2097.70 (11)$ Å^3
$Z = 8.00$
$D_x = 1.382$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 13.1–14.8°$
$\mu = 0.268$ mm^{-1}
$T = 293$ K
Long plate
0.60 × 0.45 × 0.22 mm
Cream

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: none
2391 measured reflections
1851 independent reflections
1580 observed reflections [$I > 3\sigma(I)$]

$R_{int} = 0.026$
$\theta_{max} = 26°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 12$
$l = 0 \rightarrow 29$
1 standard reflection frequency: 60 min intensity decay: 2%, correction applied

Refinement

Refinement on F
$R = 0.041$
$wR = 0.045$
$S = 1.42$
1580 reflections
159 parameters
All H-atom parameters refined, except those on C4 (riding)
$w = 1/[\sigma^2(F) + 0.001F^2]$

$(\Delta/\sigma)_{max} = 0.008$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Atomic scattering factors from Cromer & Mann (1968) for S, O, N and C atoms, and Stewart, Davidson & Simpson (1965) for H atoms

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

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

	x	y	z	U_{eq}
S1	0.17420 (7)	0.53070 (2)	0.19390 (5)	0.0516 (2)
O1	0.0789 (2)	0.58160 (6)	−0.0149 (1)	0.0580 (5)
N1	0.0573 (2)	0.59240 (7)	0.3674 (2)	0.0454 (5)
N2	−0.0119 (2)	0.62590 (7)	0.1662 (2)	0.0416 (5)
C1	0.0635 (2)	0.58910 (8)	0.2385 (2)	0.0393 (6)
C2	0.1381 (3)	0.5499 (1)	0.4298 (2)	0.0558 (7)
C3	0.2065 (3)	0.5139 (1)	0.3529 (3)	0.0603 (8)
C4	−0.0343 (3)	0.6355 (1)	0.4328 (2)	0.0603 (8)
C5	−0.0038 (2)	0.61770 (7)	0.0383 (2)	0.0406 (6)
C6	−0.1065 (2)	0.65530 (8)	−0.0398 (2)	0.0390 (6)
C7	−0.1671 (2)	0.70520 (9)	0.0088 (2)	0.0474 (6)
C8	−0.2640 (3)	0.7386 (1)	−0.0660 (3)	0.0580 (8)
C9	−0.3034 (3)	0.7221 (1)	−0.1879 (2)	0.0648 (10)
C10	−0.2438 (3)	0.6730 (1)	−0.2369 (2)	0.0653 (9)
C11	−0.1438 (3)	0.6399 (1)	−0.1639 (2)	0.0511 (7)

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

S1—C1	1.737 (2)	C2—C3	1.308 (3)
S1—C3	1.731 (2)	C5—C6	1.489 (2)
O1—C5	1.238 (2)	C6—C7	1.388 (2)
N1—C1	1.351 (2)	C6—C11	1.384 (2)
N1—C2	1.382 (2)	C7—C8	1.382 (3)
N1—C4	1.454 (2)	C8—C9	1.374 (3)
N2—C1	1.319 (2)	C9—C10	1.370 (4)
N2—C5	1.353 (2)	C10—C11	1.383 (3)
C1—S1—C3	90.7 (1)	N2—C5—C6	115.2 (2)
C2—N1—C4	123.7 (2)	O1—C5—C6	119.9 (2)
C1—N1—C4	122.0 (2)	C5—C6—C11	119.2 (2)
C1—N1—C2	114.2 (2)	C5—C6—C7	121.8 (2)
C1—N2—C5	116.5 (2)	C7—C6—C11	119.0 (2)
N1—C1—N2	120.9 (2)	C6—C7—C8	120.1 (2)
S1—C1—N2	129.4 (2)	C7—C8—C9	120.3 (2)
S1—C1—N1	109.6 (1)	C8—C9—C10	120.1 (2)
N1—C2—C3	113.9 (2)	C9—C10—C11	120.1 (2)
S1—C3—C2	111.7 (2)	C6—C11—C10	120.4 (2)
O1—C5—N2	124.9 (2)		

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *SDP* (Frenz, 1983). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELX*76 (Sheldrick, 1976). Molecular graphics: *PLUTON*93 (Spek, 1993). Software used to prepare material for publication: *PARST* (Nardelli, 1992).

We thank Professor R. F. Hudson for interesting discussions and the University of Kent for financial support.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HA1147). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1996). C**52**, 139–142

1,3-Dibenzylthiourea and 1,3-Dicyclohexylthiourea

Akilan Ramnathan,[a] Kandasamy Sivakumar,[a]† Kulandaivelu Subramanian,[a] Dravida Meerarani,[b] Krishnamoorthy Ramadas[b] and Hoong-Kun Fun[c]

[a]*Department of Physics, Anna University, Madras-600 025, India,* [b]*Centre for Agrochemical Research, SPIC Science Foundation, 110, Mount Road, Madras-600 032, India, and* [c]*X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia*

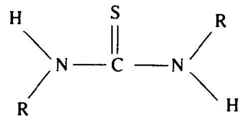
(*Received 12 May 1995; accepted 19 July 1995*)

Abstract

Crystal structures of two symmetrically substituted thiourea derivatives, 1,3-dibenzylthiourea, $C_{15}H_{16}N_2S$ (DBTU), and 1,3-dicyclohexylthiourea, $C_{13}H_{24}N_2S$ (DCHTU), are reported. One of the cyclohexane rings in DCHTU is disordered adopting two orientations separated by an angle of 44.6 (2)°. In both structures centrosymmetrically related molecules are linked by N—H···S hydrogen bonds to form dimers and weak N—H···S bonds connecting glide-related molecules are also observed in both DBTU and DCHTU.

Comment

There have been many structural studies of metal complexes of thiourea but relatively few of substituted thioureas, possibly as a result of the difficulty in obtaining suitable crystals for X-ray diffraction studies. These thioureas find applications as rubber accelerators and as intermediates for dye preparation; they are also used for the synthesis of unsymmetrical thioureas (Ramadas, Srinivasan & Janarthanan, 1993), which are very useful agrochemical intermediates. We are interested in the molecular conformations and N—H···S hydrogen bonding of substituted thiourea derivatives in the solid state. In this paper we report the crystal structures of two symmetrically substituted thiourea derivatives, namely 1,3-dibenzylthiourea (DBTU) and 1,3-dicyclohexylthiourea (DCHTU). The preparation of these compounds involves a novel and cost-effective synthetic procedure described elsewhere (Ramadas & Janarthanan, 1995). A previous report on the cell dimensions and space group of DBTU (Gilli, Michelon & Toniolo, 1968) is consistent with the results given here. The displacement ellipsoid plots of the molecules with numbering scheme are shown in Fig. 1.



DBTU: R = $CH_2C_6H_5$

DCHTU: R = C_6H_{11}

DBTU: The C1═S distance, 1.700 (1) Å, is longer than the unweighted mean value, 1.681 Å, given for C═S in thioureas by Allen, Kennard, Watson, Brammer, Orpen & Taylor (1987), but is in agreement with the values observed in other symmetrically substituted thioureas (Akilan, Sivakumar, Subramanian, Janarthanan, Ramadas & Fun, 1995*a*). The bond lengths in the two symmetric segments of the molecule show some differences (Table 2); N1—C2 and C2—C3 [1.462 (2) and 1.511 (2) Å, respectively] are slightly longer than their counterparts N2—C9 and C9—C10 [1.456 (2) and 1.507 (2) Å, respectively]. The orientations of the two benzyl groups with respect to the thiourea moiety are different and relevant torsion angles are given in Table 2; the dihedral angle between the planes of the benzyl

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† Visiting Post Doctoral Research Fellow, School of Physics, University Sains Malaysia, Malaysia.

Acta Crystallographica Section C
ISSN 0108-2701 ©1996