Crystal structure of 1-(2,6-diisopropylphenyl)-3-phenylthiourea, $C_{19}H_{24}N_2S$

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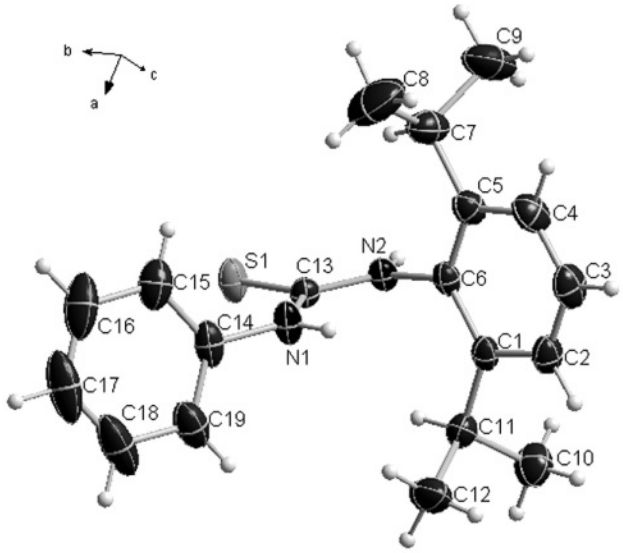

Abstract

$C_{19}H_{24}N_2S$, monoclinic, $P2_1/c$ (no. 14), a = 9.7421(7) Å, b = 15.788(1) Å, c = 12.2157(9) Å, β = 101.019(2)°, V = 1844.2 Å^3, Z = 4, $R_{gt}(F)$ = 0.0503, $wR_{ref}(F^2)$ = 0.1442, T = 273 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.18×0.20×0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.75 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, ω
$2\theta_{max}$:	52.14°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	18408, 3640
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3073
$N(param)_{refined}$:	203
Programs:	SHELX [10]

Source of material

Phenyl isothiocyanate (1 mmol) and 2,6-diisopropylaniline (1 mmol) were mixed in trichloromethane (20 mL) and refluxed for 30 minutes. The solution was kept at room temperature for 4 d. Colourless block-shaped single crystals were obtained by evaporation.

Experimental details

All H atoms were constrained to ideal geometries, with C–H = 0.93-0.98 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

Discussion

Phenylthiourea derivatives are more recognized because of their extensive biological activity in recent years, such as antiviral, antimicrobial, antidiabetics, anti-HIV, anticancer and antiviral [1-6]. In addition, phenylthioureas have also been widely used as ligands in the preparation of complexes [7-8]. According to the pharmacological applications, the title compound was synthesized. In the structure N–H···S hydrogen bonded centrosymmetric dimers are present (N···S = 3.34 Å). The dihedral angle between the best planes of the two phenyl rings in the compound is 69.42(8)°. All bond lengths in the molecule are within normal values [9].

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2A)	4*e*	0.9412	0.9158	–0.0008	0.051
H(1)	4*e*	0.7276	0.8679	0.1586	0.068
H(11)	4*e*	0.6778	0.8595	–0.0846	0.068
H(2)	4*e*	0.7096	0.6389	–0.0227	0.071
H(3)	4*e*	0.8827	0.5762	0.1034	0.085
H(4)	4*e*	1.0596	0.6557	0.2043	0.082
H(7)	4*e*	1.1032	0.8791	0.1777	0.090
H(19)	4*e*	0.4681	0.9441	0.1233	0.100
H(10A)	4*e*	0.7453	0.7747	–0.2221	0.121
H(10B)	4*e*	0.5839	0.7917	–0.2517	0.121
H(10C)	4*e*	0.6400	0.7042	–0.2013	0.121
H(15)	4*e*	0.8145	1.0078	0.3387	0.099
H(17)	4*e*	0.4371	1.0730	0.3962	0.154
H(9A)	4*e*	1.2644	0.7304	0.2161	0.167
H(9B)	4*e*	1.3260	0.8223	0.2327	0.167
H(9C)	4*e*	1.2589	0.7903	0.1129	0.167
H(12A)	4*e*	0.4934	0.7255	–0.0588	0.137
H(12B)	4*e*	0.4491	0.8181	–0.0961	0.137
H(12C)	4*e*	0.5245	0.8001	0.0270	0.137
H(18)	4*e*	0.3340	1.0100	0.2355	0.143
H(8A)	4*e*	1.0163	0.8521	0.3353	0.221
H(8B)	4*e*	1.1798	0.8529	0.3695	0.221
H(8C)	4*e*	1.0990	0.7665	0.3555	0.221
H(16)	4*e*	0.6765	1.0755	0.4491	0.138

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	4*e*	0.83830(3)	1.05889(2)	0.07689(3)	0.0732(2)	0.0355(2)	0.0793(2)	–0.0025(1)	0.0412(2)	0.0015(1)
N(2)	4*e*	0.89075(9)	0.89724(6)	0.04463(8)	0.0447(4)	0.0366(4)	0.0520(5)	–0.0023(4)	0.0211(4)	0.0014(4)
N(1)	4*e*	0.7349(1)	0.92218(6)	0.15709(9)	0.0708(5)	0.0371(5)	0.0752(6)	–0.0036(4)	0.0450(5)	–0.0016(4)
C(6)	4*e*	0.8870(1)	0.80731(7)	0.06173(9)	0.0450(5)	0.0366(5)	0.0525(6)	0.0002(4)	0.0210(4)	0.0009(4)
C(1)	4*e*	0.7785(1)	0.75936(7)	0.0003(1)	0.0485(5)	0.0418(5)	0.0558(6)	–0.0011(5)	0.0226(5)	–0.0049(5)
C(13)	4*e*	0.8212(1)	0.95426(7)	0.09441(9)	0.0420(5)	0.0385(5)	0.0451(5)	–0.0026(4)	0.0129(4)	0.0002(4)
C(11)	4*e*	0.6612(1)	0.79835(9)	–0.0832(1)	0.0578(7)	0.0497(7)	0.0619(7)	–0.0008(5)	0.0092(6)	–0.0106(5)
C(14)	4*e*	0.6540(1)	0.96946(8)	0.2216(1)	0.0823(7)	0.0372(5)	0.0693(7)	0.0025(5)	0.0469(6)	0.0057(5)
C(2)	4*e*	0.7804(1)	0.67218(8)	0.0177(1)	0.0631(7)	0.0427(6)	0.0766(8)	–0.0071(5)	0.0243(6)	–0.0064(6)
C(5)	4*e*	0.9946(1)	0.76982(8)	0.1389(1)	0.0505(6)	0.0489(6)	0.0670(7)	0.0016(5)	0.0140(5)	0.0057(6)
C(3)	4*e*	0.8839(2)	0.63454(9)	0.0929(1)	0.0835(9)	0.0377(6)	0.096(1)	0.0010(6)	0.0305(8)	0.0077(6)
C(4)	4*e*	0.9898(2)	0.68220(9)	0.1532(1)	0.0675(8)	0.0541(7)	0.0840(9)	0.0124(6)	0.0137(7)	0.0177(7)
C(7)	4*e*	1.1123(2)	0.8209(1)	0.2059(1)	0.0619(8)	0.0675(9)	0.088(1)	–0.0038(7)	–0.0080(7)	0.0109(8)
C(19)	4*e*	0.5108(2)	0.9701(1)	0.1895(2)	0.0752(8)	0.0666(9)	0.120(1)	0.0075(7)	0.0494(8)	0.0025(9)
C(10)	4*e*	0.6572(2)	0.7641(1)	–0.2004(1)	0.099(1)	0.081(1)	0.0630(8)	0.0052(9)	0.0169(8)	–0.0054(8)
C(15)	4*e*	0.7176(2)	1.0081(1)	0.3175(1)	0.120(1)	0.0633(9)	0.0710(9)	0.0034(9)	0.0372(8)	–0.0036(7)
C(17)	4*e*	0.4921(3)	1.0472(1)	0.3514(2)	0.195(2)	0.080(1)	0.147(1)	0.040(1)	0.128(1)	0.018(1)
C(9)	4*e*	1.2533(2)	0.7880(2)	0.1905(2)	0.0577(9)	0.118(2)	0.149(2)	–0.004(1)	–0.002(1)	0.018(1)
C(12)	4*e*	0.5187(2)	0.7842(1)	–0.0496(2)	0.0542(8)	0.129(2)	0.089(1)	0.0060(9)	0.0106(8)	–0.022(1)
C(18)	4*e*	0.4309(2)	1.0096(1)	0.2565(2)	0.112(1)	0.081(1)	0.191(2)	0.027(1)	0.099(1)	0.018(1)
C(8)	4*e*	1.1008(3)	0.8233(2)	0.3277(2)	0.139(2)	0.197(3)	0.100(2)	–0.051(2)	0.005(1)	–0.050(2)
C(16)	4*e*	0.6350(3)	1.0482(1)	0.3836(2)	0.210(2)	0.073(1)	0.079(1)	0.019(1)	0.068(1)	–0.0054(8)

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