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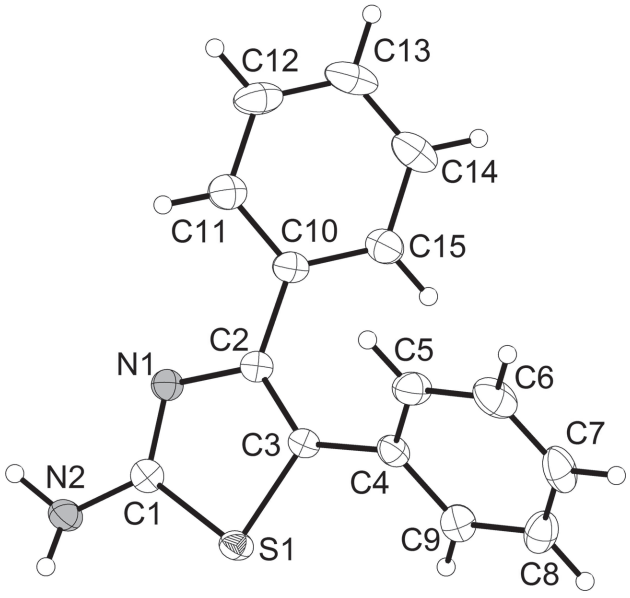
Crystal structure of 4,5-diphenylthiazol-2-amine, $C_{15}H_{12}N_2S$



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Abstract

$C_{15}H_{12}N_2S$, monoclinic, $P2_1/c$ (no. 14), $a = 6.8853(3)$ Å, $b = 23.8495(10)$ Å, $c = 7.5689(3)$ Å, $\beta = 96.585(2)°$, $V = 1234.70(9)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0506$, $wR_{ref}(F^2) = 0.1243$, $T = 100$ K.

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Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Yellow, plate, size 0.084×0.354×0.478 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.43 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω scans
$2\theta_{max}$:	61.04°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	17571, 3729
$N(param)_{refined}$:	171
Programs:	Bruker programs [7], SHELX [8]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	Site	x	y	z	U_{iso}
H(5A)	4*e*	0.5532	0.6503	0.9259	0.022
H(6A)	4*e*	0.8227	0.6937	1.0848	0.028
H(7A)	4*e*	1.1323	0.6526	1.1017	0.026
H(8A)	4*e*	1.1716	0.5676	0.9566	0.024
H(9A)	4*e*	0.9040	0.5239	0.7952	0.020
H(11A)	4*e*	0.0602	0.6389	0.5769	0.021
H(12A)	4*e*	0.0197	0.7275	0.4479	0.028
H(13A)	4*e*	0.2838	0.7742	0.3481	0.029
H(14A)	4*e*	0.5924	0.7323	0.3807	0.030
H(15A)	4*e*	0.6370	0.6437	0.5117	0.024
H(2N2)	4*e*	0.024(4)	0.448(1)	0.575(3)	0.035(6)
H(1N2)	4*e*	0.162(4)	0.415(1)	0.699(3)	0.033(6)

Source of material

2-Hydroxy-1,2-diphenylethanone (1 equiv) was dissolved in CH_2Cl_2 (70 mL), $SOCl_2$ (4 equiv), and 3 or 4 drops of DMF were added at 0°C, and the reaction was stirred for 1 h at 0°C. After completion of reaction, CH_2Cl_2 and $SOCl_2$ were removed in vacuum. Water (80 mL) and EtOAc (150 mL) were added to the residue, and the EtOAc layer was separated, dried with Na_2SO_4, filtered, and concentrated. The product (1 equiv) and thiourea (1.2 equiv) were vigorously stirred in EtOH (10 mL) at 80°C for 15 h. The progress of the reaction was monitored by TLC. After completion of the reaction, EtOH was evaporated, the precipitated crude product was filtered, dried and crystallized from ethanol to yield (70%) of the title compound ($C_{15}H_{12}N_2S$) as yellow plate crystals; mp: 214–217°C [1].

Table 3: Fractional coordinates and atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	4*e*	0.49472(6)	0.48334(2)	0.78053(5)	0.0164(2)	0.0119(2)	0.0130(2)	−0.0007(2)	−0.0027(1)	0.0009(1)
N(1)	4*e*	0.2283(2)	0.53650(6)	0.5803(2)	0.0139(7)	0.0126(6)	0.0129(6)	−0.0003(5)	0.0004(5)	−0.0006(5)
N(2)	4*e*	0.1539(2)	0.44137(6)	0.6232(2)	0.0172(8)	0.0129(7)	0.0174(7)	−0.0021(6)	−0.0030(6)	0.0018(5)
C(1)	4*e*	0.2702(3)	0.48713(7)	0.6509(2)	0.0154(8)	0.0145(7)	0.0106(7)	−0.0005(6)	0.0016(6)	−0.0009(6)
C(2)	4*e*	0.3769(2)	0.57475(7)	0.6319(2)	0.0145(8)	0.0127(7)	0.0112(7)	0.0004(6)	0.0013(6)	−0.0008(5)
C(3)	4*e*	0.5306(2)	0.55469(7)	0.7438(2)	0.0141(8)	0.0110(7)	0.0135(8)	0.0001(6)	0.0016(6)	0.0005(5)
C(4)	4*e*	0.7017(2)	0.58295(7)	0.8408(2)	0.0164(9)	0.0126(7)	0.0125(7)	−0.0023(6)	−0.0003(6)	0.0014(5)
C(5)	4*e*	0.6788(3)	0.63348(7)	0.9304(2)	0.0204(9)	0.0147(7)	0.0194(8)	0.0010(7)	−0.0015(7)	−0.0002(6)
C(6)	4*e*	0.8393(3)	0.65912(7)	1.0259(2)	0.032(1)	0.0149(8)	0.0213(9)	−0.0052(7)	−0.0019(8)	−0.0027(6)
C(7)	4*e*	1.0233(3)	0.63489(8)	1.0362(2)	0.023(1)	0.0246(9)	0.0164(8)	−0.0111(8)	−0.0020(7)	0.0010(7)
C(8)	4*e*	1.0461(3)	0.58455(8)	0.9499(2)	0.0151(9)	0.0281(9)	0.0152(8)	−0.0019(7)	0.0001(6)	0.0023(7)
C(9)	4*e*	0.8865(3)	0.55860(7)	0.8532(2)	0.0180(9)	0.0182(8)	0.0133(8)	−0.0016(7)	0.0017(6)	−0.0001(6)
C(10)	4*e*	0.3535(3)	0.63210(7)	0.5579(2)	0.0177(9)	0.0126(7)	0.0111(7)	0.0002(6)	−0.0021(6)	−0.0012(6)
C(11)	4*e*	0.1692(3)	0.65766(7)	0.5377(2)	0.0202(9)	0.0143(8)	0.0166(8)	−0.0003(6)	−0.0028(7)	−0.0035(6)
C(12)	4*e*	0.1451(3)	0.71033(7)	0.4604(2)	0.028(1)	0.0163(8)	0.0218(9)	0.0056(7)	−0.0097(8)	−0.0032(6)
C(13)	4*e*	0.3016(3)	0.73819(7)	0.4015(2)	0.041(1)	0.0131(8)	0.0176(9)	0.0006(8)	−0.0058(8)	0.0018(6)
C(14)	4*e*	0.4844(3)	0.71327(8)	0.4208(2)	0.035(1)	0.0173(8)	0.0220(9)	−0.0046(8)	0.0032(8)	0.0040(7)
C(15)	4*e*	0.5110(3)	0.66045(7)	0.4988(2)	0.0210(9)	0.0163(8)	0.0212(9)	−0.0006(7)	0.0014(7)	0.0027(6)

Experimental details

The hydrogen atoms were placed on calculated positions using a riding model (AFIX 43 option of the SHELX program [8]).

Discussion

2-Aminothiazole derivatives are greatly used as structural motifs in pharmaceutical chemistry because of their wide range of applications in drug development. Several reports on the application of 2-aminothiazoles in the treatment of a diverse range of different diseases like Alzheimer's disease [2], chronic pain [3], cancer [4] , Huntington's disease [5] and anticonvulsant [6] appeared in the scientific literature over the last few years.

In the title compound, $C_{15}H_{12}N_2S$, the asymmetric unit contains one crystallographic independent molecule. The thiazol ring (N1/S1/C1—C3) makes the dihedral angles 49.39(2)° and 39.91 (3)° with phenyl ring (C4—C9) and phenyl ring (C10—C15), respectively (figure). The structure shows one classical hydrogen bond crystallographic independent between N2—H2N2$\cdots$N1 with the symmetry code: $-x$, $-y+1$, $-z+1$. The title molecules are pairwise connected by two symmetry related hydrogen bond.

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