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1-(10*H*-Phenothiazin-2-yl)ethanone

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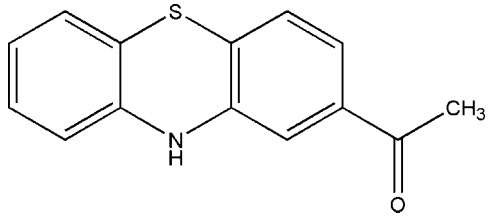
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.108; data-to-parameter ratio = 20.9.

In the title compound, $C_{14}H_{11}NOS$, the thiazine ring adopts a slightly distorted boat conformation. The dihedral angle between the mean planes of the two benzene rings is 20.2 (9)°. An intermolecular N—H···O hydrogen bond and a weak C—H···π interaction occur in the crystal, creating a two-dimensional network parallel to the *bc* plane.

Related literature

For applications of phenothiazines in drugs and medicine, see: Miller *et al.* (1999); Wermuth (2003); Wang *et al.* (2008); Lam *et al.* (2001); Kojilo *et al.* (2001). For related structures, see: Bell *et al.* (1968); McDowell (1969, 1970, 1975, 1976, 1978, 1980); Chu & Van der Helm (1974, 1975, 1977)); Phelps & Cordes (1974, 1975); Harrison *et al.* (2007); Wang *et al.* (2009). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{14}H_{11}NOS$
M_r = 241.30
Monoclinic, $P2_1/c$
a = 14.3445 (18) Å
b = 5.5425 (7) Å
c = 15.694 (2) Å
β = 114.494 (2)°
V = 1135.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 100 K
0.55 × 0.55 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.868, T_{max} = 0.974
8194 measured reflections
3331 independent reflections
2828 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.108
S = 1.04
3331 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

*Cg*3 is the centroid of the C7–C12 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H15···O1^{i}	0.829 (18)	2.198 (18)	3.0042 (15)	164.3 (17)
C9—H14···*Cg*3^{ii}	0.93	2.64	3.306 (7)	130

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

JPJ thanks Dr Matthias Zeller and the YSU Department of Chemistry for their assistance with the data collection. The diffractometer was funded by NSF grant 0087210, by Ohio Board of Regents grant CAP-491, and by YSU. BN thanks Mangalore University for the research facilities and the UGC for financial assistance through a SAP chemical grant. HSY thanks the University of Mysore for sabbatical leave.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2662).

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1-(10*H*-Phenothiazin-2-yl)ethanone

Jerry P. Jasinski, Albert E. Pek, Prakash S. Nayak, B. Narayana and H. S. Yathirajan

S1. Comment

Phenothiazine is a well known heterocycle. The phenothiazine structure occurs in many synthetic dyes, electroluminescent materials (Miller *et al.*, 1999) and drugs, especially various antipsychotic drugs, *e.g.* chlorpromazine and antihistaminic drugs, *e.g.* promethazine (Wermuth, 2003). Recently, researchers have found new applications for phenothiazine derivatives in medicine related to antitubercular (Wang *et al.*, 2008) and antitumor activities (Lam *et al.*, 2001). A review of various aspects of phenothiazines has been published (Kojilo *et al.*, 2001). The crystal and molecular structure studies of phenothiazine (Bell *et al.*, 1968), chlorpromazine, thiethylperazine, thioridazine, phenothiazine, perphenazine, trifluperazine hydrochloride (McDowell, 1969, 1970, 1975, 1976, 1978, 1980), *N*-methylphenothiazine, *N*-ethylphenothiazine, *N*-benzylphenothiazine (Chu & Van der Helm, 1974, 1975, 1977), triflupromazine, 2-methoxyphenothiazine (Phelps & Cordes, 1974, 1975), Phenothiazine-picric acid (1/1) (Harrison *et al.*, 2007) and 10-acetyl-10*H*-phenothiazine 5-oxide (Wang *et al.*, 2009) have been reported. In view of the importance of phenothiazines, this paper reports the crystal structure of the title compound, 1-(10*H*-phenothiazin-2-yl)ethanone.

The title compound, $C_{14}H_{11}NOS$, consists of benzene and phenyl-ethanone rings fused to a thiazine ring which adopts a slightly distorted boat conformation with puckering parameters Q, θ and φ of 0.371 (4) Å, 100.1 (2)° and 181.457 (4)°, respectively (Cremer & Pople, 1975) (Fig. 1). For an ideal boat Phi= k *x* 60. The dihedral angles between the mean planes of the two 6-membered benzene rings, and thiazine ring are 10.5 (5) and 10.3 (6)°. An N—H···O intermolecular hydrogen bond and a weak C—H···π interaction (Table 1) contributes to crystal packing creating a 2-D network structure parallel to the *bc* plane (Fig. 2).

S2. Experimental

1-(10*H*-Phenothiazin-3-yl)ethanone was obtained from Aldrich and it was crystallized from a dimethylformamide solution (m.p. 455–457 K)

S3. Refinement

The H15 atom bonded to N1 was freely refined. All of the other H atoms were placed in their calculated positions and then refined using the riding model with C—H lengths of 0.93 Å (CH), or 0.96 Å (CH_3). Isotropic displacement parameters for these atoms were set to 1.18–1.20 (CH) or 1.51 (CH_3) times U_{eq} of the parent atom.

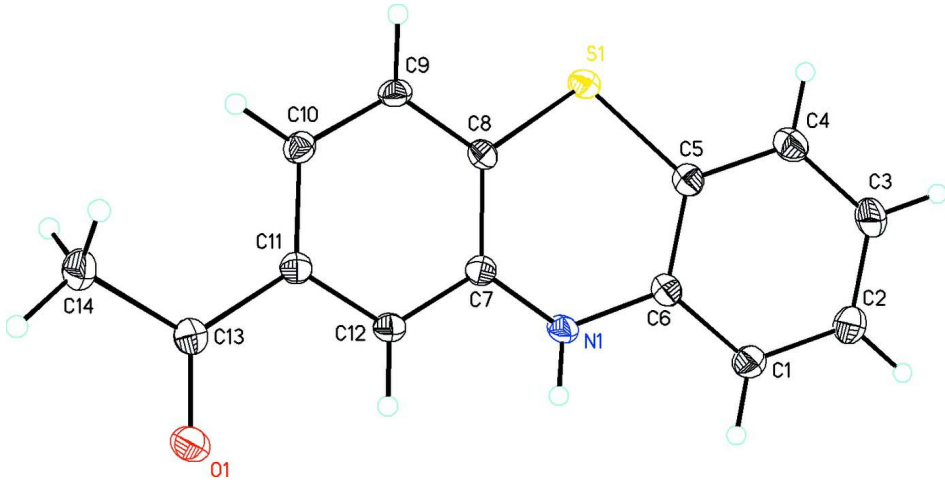

Figure 1

Molecular structure of $C_{14}H_{11}N$ O S, showing the atom labeling scheme and 50% probability displacement ellipsoids.

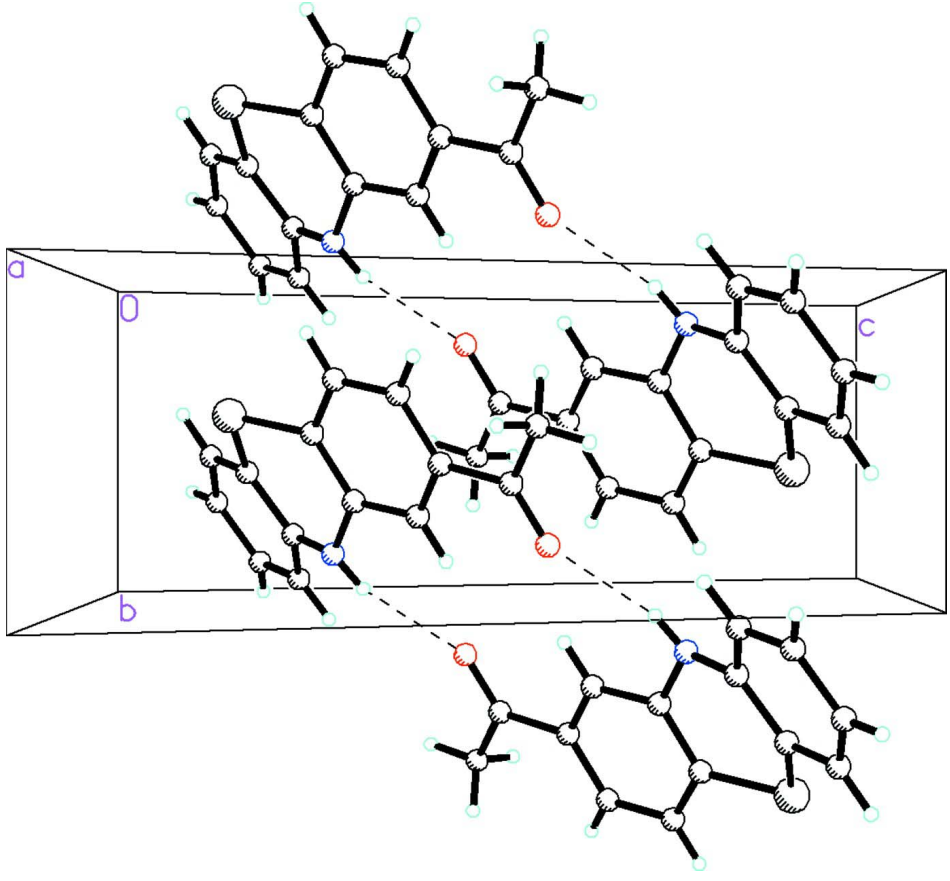

Figure 2

Packing diagram of the title compound viewed down the *a* axis. Dashed lines indicate N—H···O hydrogen bonding creating a 2-D network structure parallel to the *bc* plane.

1-(10*H*-Phenothiazin-2-yl)ethanone

Crystal data

$C_{14}H_{11}NOS$
$M_r = 241.30$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.3445\ (18)$ Å
$b = 5.5425\ (7)$ Å
$c = 15.694\ (2)$ Å
$\beta = 114.494\ (2)°$
$V = 1135.4\ (2)$ Å^3
$Z = 4$
$F(000) = 504$
$D_x = 1.412$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2781 reflections
$\theta = 2.6–30.6°$
$\mu = 0.27$ mm^{-1}
$T = 100$ K
Plate, orange
0.55 × 0.55 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.868$, $T_{max} = 0.974$
8194 measured reflections
3331 independent reflections
2828 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 31.2°$, $\theta_{min} = 1.6°$
$h = -20\rightarrow18$
$k = -8\rightarrow7$
$l = -21\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.108$
$S = 1.04$
3331 reflections
159 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.4353P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
S1	0.26560 (3)	0.41617 (6)	0.15897 (2)	0.01761 (10)
O1	0.65447 (8)	0.81327 (19)	0.54988 (7)	0.0213 (2)
N1	0.30331 (9)	0.8588 (2)	0.28579 (8)	0.0165 (2)

C11	0.55267 (10)	0.5672 (2)	0.42245 (9)	0.0140 (2)
C8	0.37282 (10)	0.4732 (2)	0.26461 (9)	0.0139 (2)
C12	0.47152 (10)	0.7316 (2)	0.39393 (9)	0.0143 (2)
H11	0.4778	0.8723	0.4282	0.017*
C13	0.64777 (10)	0.6258 (2)	0.50679 (9)	0.0158 (3)
C5	0.17254 (10)	0.5996 (2)	0.17352 (9)	0.0158 (3)
C7	0.38142 (10)	0.6876 (2)	0.31481 (9)	0.0137 (2)
C10	0.54264 (10)	0.3531 (2)	0.37268 (9)	0.0148 (2)
H9	0.5960	0.2420	0.3918	0.018*
C6	0.20076 (10)	0.8030 (2)	0.23161 (9)	0.0154 (2)
C14	0.73624 (11)	0.4520 (3)	0.53624 (10)	0.0212 (3)
H13A	0.7645	0.4522	0.4905	0.032*
H13B	0.7127	0.2927	0.5412	0.032*
H13C	0.7879	0.5003	0.5959	0.032*
C2	0.02171 (11)	0.9054 (3)	0.17891 (11)	0.0228 (3)
H2	−0.0286	1.0098	0.1799	0.027*
C4	0.06974 (11)	0.5477 (3)	0.12089 (10)	0.0201 (3)
H4	0.0514	0.4087	0.0845	0.024*
C1	0.12425 (11)	0.9539 (3)	0.23424 (10)	0.0199 (3)
H1	0.1420	1.0881	0.2733	0.024*
C3	−0.00598 (11)	0.7028 (3)	0.12236 (10)	0.0231 (3)
H3	−0.0747	0.6703	0.0856	0.028*
C9	0.45264 (10)	0.3070 (2)	0.29454 (9)	0.0150 (2)
H14	0.4456	0.1634	0.2618	0.018*
H15	0.3129 (13)	0.971 (3)	0.3234 (12)	0.018 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01602 (18)	0.01739 (18)	0.01652 (17)	−0.00026 (12)	0.00384 (13)	−0.00450 (11)
O1	0.0212 (5)	0.0192 (5)	0.0192 (5)	−0.0004 (4)	0.0041 (4)	−0.0037 (4)
N1	0.0149 (5)	0.0108 (5)	0.0202 (5)	0.0003 (4)	0.0036 (4)	−0.0024 (4)
C11	0.0145 (6)	0.0128 (6)	0.0148 (5)	−0.0002 (4)	0.0061 (5)	0.0008 (4)
C8	0.0137 (6)	0.0131 (6)	0.0150 (5)	−0.0022 (4)	0.0059 (5)	−0.0003 (4)
C12	0.0162 (6)	0.0112 (6)	0.0156 (6)	−0.0004 (4)	0.0067 (5)	−0.0008 (4)
C13	0.0159 (6)	0.0159 (6)	0.0160 (6)	−0.0009 (5)	0.0070 (5)	0.0015 (5)
C5	0.0155 (6)	0.0153 (6)	0.0150 (6)	0.0007 (5)	0.0045 (5)	0.0019 (4)
C7	0.0147 (6)	0.0113 (6)	0.0155 (6)	−0.0003 (5)	0.0065 (5)	0.0012 (4)
C10	0.0150 (6)	0.0124 (6)	0.0177 (6)	0.0014 (5)	0.0074 (5)	0.0012 (5)
C6	0.0147 (6)	0.0142 (6)	0.0154 (6)	−0.0003 (5)	0.0042 (5)	0.0018 (4)
C14	0.0158 (7)	0.0205 (7)	0.0233 (7)	0.0024 (5)	0.0041 (6)	0.0005 (5)
C2	0.0164 (7)	0.0238 (7)	0.0252 (7)	0.0043 (5)	0.0055 (6)	−0.0004 (5)
C4	0.0189 (7)	0.0203 (7)	0.0177 (6)	−0.0022 (5)	0.0043 (5)	−0.0019 (5)
C1	0.0181 (7)	0.0179 (7)	0.0219 (6)	0.0019 (5)	0.0063 (6)	−0.0020 (5)
C3	0.0141 (6)	0.0273 (8)	0.0225 (7)	−0.0005 (5)	0.0022 (5)	−0.0011 (6)
C9	0.0175 (6)	0.0104 (6)	0.0190 (6)	−0.0007 (5)	0.0096 (5)	−0.0015 (4)

Geometric parameters (Å, º)

S1—C8	1.7606 (13)	C5—C6	1.4003 (18)
S1—C5	1.7664 (14)	C10—C9	1.3868 (18)
O1—C13	1.2216 (16)	C10—H9	0.9300
N1—C7	1.3930 (16)	C6—C1	1.3939 (18)
N1—C6	1.3948 (17)	C14—H13A	0.9600
N1—H15	0.829 (18)	C14—H13B	0.9600
C11—C10	1.3946 (18)	C14—H13C	0.9600
C11—C12	1.3980 (18)	C2—C3	1.384 (2)
C11—C13	1.4903 (18)	C2—C1	1.390 (2)
C8—C9	1.3908 (18)	C2—H2	0.9300
C8—C7	1.4026 (18)	C4—C3	1.393 (2)
C12—C7	1.3932 (18)	C4—H4	0.9300
C12—H11	0.9300	C1—H1	0.9300
C13—C14	1.5051 (19)	C3—H3	0.9300
C5—C4	1.3891 (19)	C9—H14	0.9300
C8—S1—C5	100.77 (6)	C1—C6—N1	119.56 (12)
C7—N1—C6	123.39 (11)	C1—C6—C5	118.93 (12)
C7—N1—H15	113.9 (12)	N1—C6—C5	121.51 (12)
C6—N1—H15	115.0 (12)	C13—C14—H13A	109.5
C10—C11—C12	119.76 (12)	C13—C14—H13B	109.5
C10—C11—C13	121.79 (12)	H13A—C14—H13B	109.5
C12—C11—C13	118.44 (11)	C13—C14—H13C	109.5
C9—C8—C7	120.20 (12)	H13A—C14—H13C	109.5
C9—C8—S1	118.33 (10)	H13B—C14—H13C	109.5
C7—C8—S1	121.34 (10)	C3—C2—C1	120.39 (13)
C7—C12—C11	120.84 (12)	C3—C2—H2	119.8
C7—C12—H11	119.6	C1—C2—H2	119.8
C11—C12—H11	119.6	C5—C4—C3	120.36 (13)
O1—C13—C11	120.67 (12)	C5—C4—H4	119.8
O1—C13—C14	120.76 (12)	C3—C4—H4	119.8
C11—C13—C14	118.55 (12)	C2—C1—C6	120.52 (13)
C4—C5—C6	120.19 (12)	C2—C1—H1	119.7
C4—C5—S1	118.48 (10)	C6—C1—H1	119.7
C6—C5—S1	121.18 (10)	C2—C3—C4	119.54 (13)
N1—C7—C12	119.68 (11)	C2—C3—H3	120.2
N1—C7—C8	121.47 (12)	C4—C3—H3	120.2
C12—C7—C8	118.83 (12)	C10—C9—C8	120.71 (12)
C9—C10—C11	119.62 (12)	C10—C9—H14	119.6
C9—C10—H9	120.2	C8—C9—H14	119.6
C11—C10—H9	120.2		
C5—S1—C8—C9	159.37 (10)	C12—C11—C10—C9	0.86 (18)
C5—S1—C8—C7	−24.72 (12)	C13—C11—C10—C9	−179.90 (11)
C10—C11—C12—C7	−1.68 (18)	C7—N1—C6—C1	156.10 (12)
C13—C11—C12—C7	179.06 (11)	C7—N1—C6—C5	−24.60 (19)

C10—C11—C13—O1	−179.23 (12)	C4—C5—C6—C1	−1.17 (19)
C12—C11—C13—O1	0.02 (18)	S1—C5—C6—C1	174.31 (10)
C10—C11—C13—C14	2.26 (18)	C4—C5—C6—N1	179.53 (13)
C12—C11—C13—C14	−178.50 (12)	S1—C5—C6—N1	−5.00 (18)
C8—S1—C5—C4	−158.90 (11)	C6—C5—C4—C3	2.7 (2)
C8—S1—C5—C6	25.55 (12)	S1—C5—C4—C3	−172.88 (11)
C6—N1—C7—C12	−156.23 (12)	C3—C2—C1—C6	1.8 (2)
C6—N1—C7—C8	25.55 (19)	N1—C6—C1—C2	178.23 (13)
C11—C12—C7—N1	−177.47 (11)	C5—C6—C1—C2	−1.1 (2)
C11—C12—C7—C8	0.80 (18)	C1—C2—C3—C4	−0.3 (2)
C9—C8—C7—N1	179.12 (11)	C5—C4—C3—C2	−2.0 (2)
S1—C8—C7—N1	3.28 (17)	C11—C10—C9—C8	0.82 (19)
C9—C8—C7—C12	0.89 (18)	C7—C8—C9—C10	−1.71 (19)
S1—C8—C7—C12	−174.95 (9)	S1—C8—C9—C10	174.25 (10)

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C7–C12 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H15···O1^{i}	0.829 (18)	2.198 (18)	3.0042 (15)	164.3 (17)
C9—H14···*Cg*3^{ii}	0.93	2.64	3.306 (7)	130

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