$\Delta\rho_{max} = 1{\cdot}03$ (3) and $\Delta\rho_{min} = -0{\cdot}28$ (3) e Å^{-3} on final difference map. Atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974) and programs used were those of Enraf–Nonius (1982) *SDP*.* Table 1 gives the atom coordinates and Table 2 selected bond distances and angles. Fig. 1 shows the molecule with the numbering scheme.

Related literature. The title compound has been considered to be both acyclic (Moran & Reider, 1969) and cyclic (Schmidpeter & Stoll, 1971). The present study confirms the latter conformation.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43961 (43 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

We thank the National Science Foundation, the State of Arkansas, the Research Corporation, and the Natural Sciences and Engineering Research Council of Canada for financial support.

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Structure of 3,5-Diphenyl-4*H*-1,2,4,6-thiatriazine 1-Oxide

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Abstract. $C_{14}H_{11}N_3OS$, $M_r = 269{\cdot}3$, orthorhombic, *Pbca*, $a = 15{\cdot}682$ (4), $b = 8{\cdot}872$ (2), $c = 18{\cdot}062$ (5) Å, $V = 2513$ (2) Å^3, $Z = 8$, $D_x = 1{\cdot}42$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71073$ Å, $\mu = 2{\cdot}40$ cm^{-1}, $F(000) = 1120$, $T = 293$ K, $R = 0{\cdot}044$ for 838 unique observed reflections. The N_3C_2 portion of the ring is planar within $\pm 0{\cdot}06$ Å; the S atom is 0·549 (2) Å out of this plane. The S–N bonds average 1·677 (5) Å and the NSN angle is 103·2 (2)°.

Experimental. Compound prepared by the hydrolysis of 3,5-diphenyl-1,2,4,6-thiatriazine 1-chloride in wet acetonitrile. $S(O)N_3C_2(C_6H_5)_2$ crystals obtained from acetonitrile solutions. Colorless needle data crystal $0{\cdot}14 \times 0{\cdot}12 \times 0{\cdot}50$ mm mounted on glass fiber. Intensities measured with an Enraf–Nonius CAD-4 diffractometer using ω–2θ scans of 4 to 16° min^{-1} in θ. Unit cell determined from least-squares analysis of angle data for 25 reflections with $16 < 2\theta < 20°$. Analytical absorption correction based on crystal shape varied from 0·98 to 1·00. Data collected to $(\sin\theta)/\lambda$ of 0·62 Å^{-1}, $-10 \le h \le 0$, $0 \le k \le 19$, $0 \le l \le 22$. Three standard reflections ($\bar{3}23$, $\bar{2}35$, $1\bar{6}0$) varied $\pm 3{\cdot}0\%$ over 19·8 h of data collection; the contribution of each standard to the decay correction was weighted according to the relative distance between reciprocal-lattice points. 2459 reflections measured, 1621 reflections with $I < 3\sigma(I)$ considered unobserved. Solved by direct methods using *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) and Fourier methods. Full-matrix least squares minimized $\sum w(\Delta F)^2$. H atoms constrained to idealized (C–H = 0·95; N–H = 0·93 Å) positions with isotropic $B = 1{\cdot}2 \times B$ of bonded C or N atom. All non-H atoms refined anisotropically for a total of 172 variables. $R = 0{\cdot}044$, $wR = 0{\cdot}050$, $S = 1{\cdot}18$, where non-Poisson

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Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters for the non-H atoms*

	x	*y*	*z*	B_{eq}(Å^2)
S	0·4936 (1)	0·2956 (2)	0·13061 (7)	3·98 (3)
O	0·5799 (2)	0·3388 (4)	0·1058 (2)	4·19 (9)
N(1)	0·4418 (3)	0·4567 (5)	0·1489 (2)	4·0 (1)
N(2)	0·4439 (3)	0·2305 (5)	0·0551 (2)	4·0 (1)
N(3)	0·4047 (3)	0·4779 (5)	0·0233 (2)	3·0 (1)
C(1)	0·4127 (3)	0·5349 (6)	0·0949 (3)	3·3 (1)
C(2)	0·4128 (3)	0·3256 (6)	0·0091 (3)	3·3 (1)
C(3)	0·3808 (3)	0·6904 (6)	0·1091 (3)	3·1 (1)
C(4)	0·3396 (3)	0·7763 (7)	0·0561 (3)	3·8 (1)
C(5)	0·3133 (4)	0·9199 (7)	0·0738 (3)	4·3 (1)
C(6)	0·3272 (4)	0·9781 (6)	0·1432 (3)	4·3 (1)
C(7)	0·3684 (4)	0·8954 (7)	0·1956 (3)	4·5 (2)
C(8)	0·3951 (4)	0·7513 (7)	0·1783 (3)	4·1 (1)
C(9)	0·3819 (3)	0·2731 (6)	−0·0647 (3)	3·1 (1)
C(10)	0·3190 (4)	0·3465 (7)	−0·1034 (3)	3·7 (1)
C(11)	0·2918 (4)	0·2902 (7)	−0·1716 (3)	4·1 (1)
C(12)	0·3281 (4)	0·1598 (7)	−0·1982 (3)	4·6 (2)
C(13)	0·3904 (4)	0·0881 (7)	−0·1597 (3)	5·0 (2)
C(14)	0·4168 (4)	0·1410 (7)	−0·0916 (3)	4·2 (1)

Anisotropically refined atoms are given in the form of the equivalent isotropic thermal parameter defined as $B_{eq} = \frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

Table 2. *Selected bond distances* (Å) *and bond angles* (°) *and their e.s.d.'s.*

S	O	1·476 (4)		N(3)	C(1)	1·393 (6)	
S	N(1)	1·678 (5)		N(3)	C(2)	1·382 (6)	
S	N(2)	1·675 (4)		C(1)	C(3)	1·490 (8)	
N(1)	C(1)	1·281 (6)		C(2)	C(9)	1·492 (7)	
N(2)	C(2)	1·281 (6)					
O	S	N(1)	106·5 (2)	N(1)	C(1)	N(3)	122·8 (5)
O	S	N(2)	105·6 (2)	N(1)	C(1)	C(3)	119·3 (5)
N(1)	S	N(2)	103·2 (2)	N(3)	C(1)	C(3)	117·7 (5)
S	N(1)	C(1)	118·9 (4)	N(2)	C(2)	N(3)	124·0 (5)
S	N(2)	C(2)	118·6 (4)	N(2)	C(2)	C(9)	119·8 (5)
C(1)	N(3)	C(2)	121·3 (5)	N(3)	C(2)	C(9)	116·2 (5)

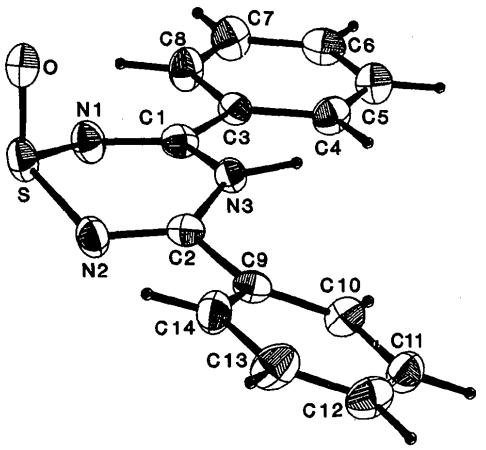

Fig. 1. *ORTEP* diagram (Johnson, 1976) and atom-numbering scheme. Non-H ellipsoids at 30% probability level, H atoms given arbitrary radii.

$w^{-1} = [\sigma^2(I) + 0{\cdot}0025I^2]/4F^2$. Final $(\Delta/\sigma)_{max} < 0{\cdot}01$, $\Delta\rho_{max} = 0{\cdot}20$ (4) and $\Delta\rho_{min} = -0{\cdot}25$ (4) e Å^{-3} on final difference map. Atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974) and programs used were those of Enraf–Nonius (1982) *SDP*.* Table 1 gives the atom coordinates and Table 2 selected bond distances and angles. Fig. 1 shows the molecule with the numbering scheme.

Related literature. The structures of 4*H*-TTA (TTA = 3,5-diphenyl-1,2,4,6-thiatriazine) and the TTA^+ cation have been reported (Boere, Cordes, Hayes, Oakley, Reed & Pennington, 1986), as have the structures of $(TTA)_2$ (Hayes, Oakley, Cordes & Pennington, 1985) and TTA 1-chloride (Cordes, Hayes, Josephy, Koenig, Oakley & Pennington, 1984). Two other molecules containing the thiatriazine ring [$N(^iPr)_2$ bonded to S atoms, Cl or SPh to the C atoms] have also been reported (Kálmán, Argay, Fischer & Rembarz, 1979).

We thank the National Science Foundation, the State of Arkansas, the Research Corporation, and the Natural Sciences and Engineering Research Council of Canada for financial support.

* Lists of structure factors, distances and angles within the phenyl rings, and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43962 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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