Related literature. Other structures exhibiting long C—C bonds due to crowding can be found in Kartt, Beckhaus, Lindner & Ruchart (1983).

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Structure of 1-Iodo-3,5-diphenyl-1λ^4,2,4,6-thiatriazine

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Abstract. $C_{14}H_{10}IN_3S$, $M_r = 379{\cdot}2$, monoclinic, $C2/c$, $a = 24{\cdot}527\ (3)$, $b = 5{\cdot}117\ (2)$, $c = 22{\cdot}495\ (3)$ Å, $\beta = 93{\cdot}85\ (1)°$, $V = 2817\ (2)$ Å^3, $Z = 8$, $D_x = 1{\cdot}79$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71073$ Å, $\mu = 23{\cdot}8$ cm^{-1}, $F(000) = 1472$, $T = 293$ K, $R = 0{\cdot}031$ for 1524 unique observed reflections. The N_3C_2 ring segment is planar within 0·048 (5) Å and the S atom is displaced 0·256 (1) Å from this plane. All of the atoms of the molecule except the I atom are planar within 0·139 (4) Å. The S—I bond distance of 2·665 (2) Å is 0·3 Å longer than value for an S—I single bond.

Experimental. Compound prepared by the reaction of elemental iodine with the dimer of 3,5-diphenyl-1,2,4,6-thiatriazine. Crystals obtained from acetonitrile solutions. Black platelet data crystal 0·08 × 0·26 × 0·58 mm mounted on a glass fiber. Density not measured. Intensities measured with an Enraf–Nonius CAD-4 diffractometer using variable-speed (3 to 17° min^{-1}) ω–2θ scans. Unit cell determined from least squares of angle data for 25 reflections with $16 < 2\theta < 24°$. Analytical absorption correction based on crystal shape varied from 0·66 to 1·00. Data collected to $\sin\theta/\lambda$ of 0·60 Å^{-1}, $0 \le h \le 29$, $-6 \le k \le 0$, $-26 \le l \le 26$. Four standard reflections (0,0,$\bar{1}$0, 10,0,0, 0,0,10, 0$\bar{2}$0) varied 4·4% over 26·9 h of data collection; anisotropic-drift correction applied. 3152 reflections measured, 3006 unique ($R_{int} = 0{\cdot}03$), 1555 reflections with $I < 3\sigma(I)$ considered unobserved. Solved by Patterson and Fourier methods. Full-matrix least squares minimized $\sum w(\Delta F)^2$. H atoms constrained to idealized (C—H = 0·95 Å) positions with isotropic $B = 1{\cdot}2 \times B$ of bonded C atom. All non-H atoms refined anisotropically for a total of 172 variables. $R = 0{\cdot}031$, $wR = 0{\cdot}038$, and $S = 1{\cdot}22$, where non-Poisson $w^{-1} = [\sigma^2(I) + 0{\cdot}0016I^2]/4F^2$. Final $(\Delta/\sigma)_{max} < 0{\cdot}01$, $\Delta\rho_{max} = 0{\cdot}56\ (5)$ and $\Delta\rho_{min} = -0{\cdot}52\ (5)$ e Å^{-3} on final difference map. Atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974); programs used those of Enraf–Nonius (1982) *SDP* package. Table 1 gives atom coordinates and Table 2 gives selected bond distances and angles.* Fig. 1 gives the atom numbering.

* Lists of structure factors and anisotropic temperature factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42792 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *for the non-*H *atoms*

	x	y	z	B_{eq}
I	0·68923 (2)	−0·0669 (1)	0·03026 (2)	5·93 (1)
S	0·61496 (5)	0·2012 (3)	0·08634 (6)	4·53 (3)
N(1)	0·6402 (2)	0·212 (1)	0·1539 (2)	4·5 (1)
N(2)	0·5637 (2)	0·0065 (9)	0·0805 (2)	4·5 (1)
N(3)	0·5890 (2)	−0·1659 (9)	0·1776 (2)	4·0 (1)
C(1)	0·6267 (2)	0·017 (1)	0·1899 (2)	3·5 (1)
C(2)	0·6565 (2)	0·010 (1)	0·2490 (2)	3·4 (1)
C(3)	0·6456 (2)	−0·183 (1)	0·2893 (2)	4·5 (1)
C(4)	0·6748 (2)	−0·196 (1)	0·3441 (2)	5·3 (1)
C(5)	0·7150 (2)	−0·015 (1)	0·3583 (2)	4·9 (1)
C(6)	0·7259 (2)	0·178 (1)	0·3190 (3)	5·1 (1)
C(7)	0·6973 (2)	0·194 (1)	0·2643 (2)	4·6 (1)
C(8)	0·5576 (2)	−0·154 (1)	0·1264 (2)	3·6 (1)
C(9)	0·5117 (2)	−0·342 (1)	0·1202 (2)	4·0 (1)
C(10)	0·5025 (2)	−0·513 (1)	0·1665 (2)	4·6 (1)
C(11)	0·4605 (2)	−0·692 (1)	0·1601 (3)	5·1 (1)
C(12)	0·4276 (2)	−0·703 (1)	0·1076 (3)	5·6 (2)
C(13)	0·4367 (3)	−0·533 (1)	0·0623 (3)	5·9 (2)
C(14)	0·4785 (2)	−0·353 (1)	0·0678 (3)	5·1 (1)

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

Table 2. *Selected bond lengths* (Å) *and bond angles* (°)

S	I	2·665 (2)		N(3)	C(8)		1·344 (6)
S	N(1)	1·604 (4)		C(1)	C(2)		1·475 (7)
S	N(2)	1·603 (4)		C(8)	C(9)		1·481 (7)
N(1)	C(1)	1·341 (6)		C–C phenyl av.			1·380
N(2)	C(8)	1·336 (6)		C–C phenyl range			1·363–1·398
N(3)	C(1)	1·331 (6)					
I	S	N(1)	103·5 (2)	N(2)	C(8)	N(3)	127·1 (5)
I	S	N(2)	101·4 (2)	N(1)	C(1)	C(2)	115·7 (4)
N(1)	S	N(2)	110·5 (2)	N(3)	C(1)	C(2)	117·8 (4)
S	N(1)	C(1)	116·8 (4)	N(2)	C(8)	C(9)	116·7 (4)
S	N(2)	C(8)	116·5 (4)	N(3)	C(8)	C(9)	116·1 (5)
C(1)	N(3)	C(8)	119·7 (4)	C–C–C phenyl range			119·1–121·1
N(1)	C(1)	N(3)	126·5 (5)				

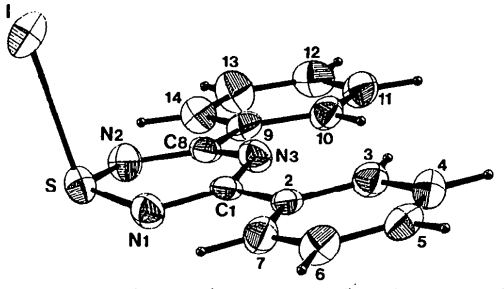

Fig. 1. *ORTEP*II diagram (Johnson, 1976) and atom-numbering scheme. Non-H ellipsoids at 30% probability level, H atoms given arbitrary radii.

Related literature. Structures of four other derivatives of 3,5-diphenyl-1,2,4,6-thiatriazine have been reported: $Ph_2C_2SN_3^{\ddagger}.PF_6^-$ and $Ph_2C_2SN_3H$ (Boeré, Cordes, Hayes, Oakley, Reed & Pennington, 1986), $Ph_2C_2SN_3Cl$ (Cordes, Hayes, Josephy, Koenig, Oakley & Pennington, 1984) and $(Ph_2C_2SN_3)_2$ (Hayes, Oakley, Cordes & Pennington, 1985). Three other structures of molecules containing the thiatriazine ring have been published (Kálmań, Argay, Fischer, Rembarz & Voss, 1977; Kálmań, Argay, Fischer & Rembarz, 1979). Structures with S–I bonds include the covalent bond of 2·347 (6) Å in the S_7I^+ cation (Passmore, Taylor, Whidden & White, 1976) and the S···I contacts of 2·6–2·7 Å in adduct molecules (Lin & Hope, 1972; Ahisen & Stromme, 1974; Burford, Chivers, Hojo, Laidlaw, Richardson & Trsic, 1985).

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