Related literature. This compound is one of a series of TAG compounds being studied by this laboratory. Previous structure determinations for different TAG salts in this series are reported by Okaya & Pepinsky (1957), Bracuti (1979, 1983) and Choi & Prince (1979).

The X-ray diffraction data presented were obtained by the Molecular Structure Corp., College Station, Texas, under Contract DAAG PO 84–046.

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Structure of 1,1-Dichloro-3,5-diphenyl-4*H*-1,2,4,6-selenatriazine

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(*Received* 6 *June* 1986; *accepted* 25 *June* 1986)

Abstract. $C_{14}H_{11}Cl_2N_3Se$, $M_r = 371{\cdot}1$, monoclinic, $P2_1/n$, $a = 10{\cdot}488\ (4)$, $b = 10{\cdot}217\ (4)$, $c = 14{\cdot}006\ (5)$ Å, $\beta = 99{\cdot}77\ (3)°$, $V = 1479\ (2)$ Å^3, $Z = 4$, $D_x = 1{\cdot}67$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71073$ Å, $\mu = 28{\cdot}7$ cm^{-1}, $F(000) = 736$, $T = 293$ K, $R = 0{\cdot}039$ for 1709 unique observed reflections. The SeNCNCN ring is in a boat conformation with the Se atom displaced 0·348 (1) Å and the opposite N atom (which is bonded to an H atom) displaced 0·13 (1) Å from the plane of the boat bottom. The phenyl rings are twisted 27·9 (5) and 30·0 (5)° with respect to the latter plane.

Experimental. Compound prepared by the reaction of $SeCl_4$ and $NH_2C(Ph)NC(Ph)NH_2^+Cl^-$. Crystals obtained from acetonitrile solutions. Yellow platelet data crystal 0·18 × 0·24 × 0·44 mm mounted on glass fiber. Density not measured. Intensities measured with an Enraf–Nonius CAD-4 diffractometer using ω–2θ scans of 4–16° min^{-1} in θ. Unit cell determined from least-squares analysis of angle data for 25 reflections with $21 < 2\theta < 24°$. Analytical absorption correction based on crystal shape varied from 0·76 to 1·00. Data collected to $\sin\theta/\lambda$ of 0·60 Å^{-1}, $0 \le h \le 12$, $0 \le k \le 12$, $-16 \le l \le 16$. Four standard reflections (501, $\bar{5}0\bar{1}$, $13\bar{6}$, 351) varied ±0·7% over 24·2 h of data collection; anisotropic drift correction applied. 2763 reflections

Table 1. *Fractional atomic coordinates and isotropic thermal parameters, with their e.s.d.'s in parentheses*

$B_{eq} = \frac{4}{3}(a^2B_{11} + b^2B_{22} + c^2B_{33} + acB_{13}\cos\beta)$.

	x	y	z	B_{eq}/B(Å)^2
Se	0·08262 (5)	0·13745 (5)	0·10430 (4)	2·710 (9)
Cl(1)	0·1163 (2)	0·3602 (2)	0·0574 (1)	4·02 (3)
Cl(2)	0·0325 (2)	−0·0872 (2)	0·1350 (1)	4·24 (3)
N(1)	0·0646 (4)	0·1837 (5)	0·2261 (3)	3·00 (9)
N(2)	0·2534 (4)	0·1020 (4)	0·1096 (3)	2·82 (9)
N(3)	0·2678 (4)	0·0843 (4)	0·2810 (3)	2·53 (8)
C(1)	0·1546 (4)	0·1442 (5)	0·2945 (3)	2·6 (1)
C(2)	0·1371 (5)	0·1621 (5)	0·3955 (3)	2·5 (1)
C(3)	0·2417 (5)	0·1823 (6)	0·4700 (4)	3·4 (1)
C(4)	0·2210 (6)	0·1995 (7)	0·5635 (4)	4·2 (1)
C(5)	0·0964 (6)	0·1939 (7)	0·5840 (4)	4·3 (1)
C(6)	−0·0061 (6)	0·1756 (6)	0·5108 (4)	4·2 (1)
C(7)	0·0136 (5)	0·1602 (6)	0·4171 (4)	3·5 (1)
C(8)	0·3166 (5)	0·0787 (5)	0·1960 (3)	2·4 (1)
C(9)	0·4557 (4)	0·0468 (5)	0·2061 (3)	2·4 (1)
C(10)	0·5410 (5)	0·0843 (6)	0·2886 (4)	3·3 (1)
C(11)	0·6712 (5)	0·0617 (7)	0·2947 (4)	4·2 (1)
C(12)	0·7179 (5)	0·0009 (7)	0·2203 (5)	4·6 (1)
C(13)	0·6336 (5)	−0·0387 (6)	0·1385 (4)	3·8 (1)
C(14)	0·5030 (5)	−0·0149 (6)	0·1308 (4)	3·2 (1)
H(N3)	0·3262	0·0488	0·3379	

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

Se–Cl(1)	2·411 (2)	N(2)–C(8)	1·300 (6)
Se–Cl(2)	2·410 (2)	N(3)–C(1)	1·376 (6)
Se–N(1)	1·811 (4)	N(3)–C(8)	1·374 (5)
Se–N(2)	1·816 (4)	C(1)–C(2)	1·468 (6)
N(1)–C(1)	1·291 (6)	C(8)–C(9)	1·479 (6)
		N(3)–H(N3)	0·99
Cl(1)–Se–Cl(2)	173·80 (5)	C(1)–N(3)–C(8)	126·5 (4)
Cl(1)–Se–N(1)	93·1 (1)	N(1)–C(1)–N(3)	125·2 (4)
Cl(1)–Se–N(2)	90·6 (1)	N(2)–C(8)–N(3)	126·4 (4)
Cl(2)–Se–N(1)	91·1 (1)	N(1)–C(1)–C(2)	118·7 (4)
Cl(2)–Se–N(2)	92·6 (1)	N(3)–C(1)–C(2)	116·1 (4)
N(1)–Se–N(2)	105·9 (2)	N(2)–C(8)–C(9)	117·9 (4)
Se–N(1)–C(1)	115·9 (3)	N(3)–C(8)–C(9)	115·7 (4)
Se–N(2)–C(8)	114·7 (3)	C(1)–N(3)–H(N3)	118·9
		C(8)–N(3)–H(N3)	114·3

measured, 2613 unique ($R_{int} = 0·04$), 904 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 $\sum w(\Delta F)^2$. Phenyl H atoms constrained to idealized (C–H = 0·95 Å) positions with isotropic $B = 1·2 \times B$ of bonded C atom. H atom bonded to N(3) was constrained to the position found on a difference map and isotropic $B = 1·2 \times B$ of N(3). All non-H atoms refined anisotropically for a total of 181 variables. $R = 0·039$, $wR = 0·049$, $S = 1·20$, where non-Poisson $w^{-1} = [\sigma^2(I) + 0·0025I^2]/4F^2$. Final $(\Delta/\sigma)_{max} < 0·01$, $\Delta\rho_{max} = 0·55$ (5) and $\Delta\rho_{min} = -0·95$ (5) 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 structural parameters and the boat-like conformation of the C_2N_3Se ring are to be compared with those found in the related C_2N_3S ring (Hayes, Oakley, Cordes & Pennington, 1985; Cordes, Hayes, Josephy, Koenig, Oakley & Pennington, 1984). There are few reports of Cl–Se–N structures; those of $Ph_3P{=}NSeCl_3$ and $(Ph_3P{=}N)_2SeCl_2$ (Roesky, Weber, Seseke, Pinkert, Noltemeyer, Clegg & Sheldrick, 1985) are the most closely related. Amendola, Gould & Post (1964) reported the structure of the six-membered heterocyclic ring $C_4H_8Se_2Cl_4$. The structural characterizations of $ClSeN_3C_2Ph_2$ and $(SeN_3C_2Ph_2)_2$ have recently been completed in our laboratories and the manuscripts are in preparation.

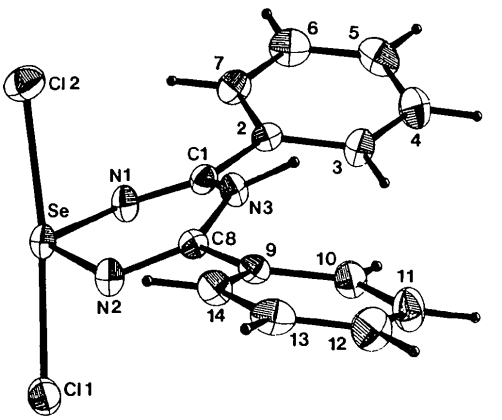

Fig. 1. *ORTEP* diagram (Johnson, 1976) and atom-numbering scheme. Non-H ellipsoids at 30% probability level, H atoms given arbitrary radii.

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 and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43188 (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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