Table 2. *Interatomic distances* (Å) *and angles* (°) *involving non-*H *atoms with e.s.d.'s in parentheses*

C(1)–C(2)	1·438 (6)	C(3)–O(7)	1·414 (4)
C(1)–C(6)	1·511 (5)	C(4)–C(5)	1·552 (6)
C(1)–O(8)	1·444 (5)	C(4)–C(9)	1·464 (4)
C(2)–C(3)	1·529 (3)	C(5)–C(6)	1·541 (4)
C(2)–O(8)	1·433 (3)	C(6)–O(7)	1·419 (4)
C(3)–C(4)	1·555 (4)	C(9)–N(10)	1·141 (4)
C(2)–C(1)–C(6)	103·3 (2)	C(3)–C(4)–C(9)	114·4 (3)
C(2)–C(1)–O(8)	59·6 (2)	C(5)–C(4)–C(9)	113·7 (2)
C(6)–C(1)–O(8)	113·1 (2)	C(4)–C(5)–C(6)	100·5 (3)
C(1)–C(2)–C(3)	103·1 (3)	C(1)–C(6)–C(5)	105·5 (2)
C(1)–C(2)–O(8)	60·4 (2)	C(1)–C(6)–O(7)	103·4 (4)
C(3)–C(2)–O(8)	113·1 (2)	C(5)–C(6)–O(7)	102·4 (2)
C(2)–C(3)–C(4)	105·3 (2)	C(3)–O(7)–C(6)	97·8 (2)
C(2)–C(3)–O(7)	102·8 (2)	C(1)–O(8)–C(2)	60·0 (2)
C(4)–C(3)–O(7)	101·4 (3)	C(4)–C(9)–N(10)	179·3 (2)
C(3)–C(4)–C(5)	101·2 (2)		

refinement procedure but not refined with the B_{eq}'s of the atoms to which they were bonded. Weighting scheme $w = 1/[\sigma^2(F) + 0{\cdot}063183F^2]$, $R = 0{\cdot}082$, $wR = 0{\cdot}085$. High R value explained by the poor quality of crystalline sample. $(\Delta/\sigma)_{max} = 0{\cdot}270$, $(\Delta/\sigma)_{min} = 0{\cdot}001$. $(\Delta/\rho)_{max} = 0{\cdot}32$ e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). All numerical calculations were performed on the 370/145 IBM computer of the Office Central de Mécanographie of Abidjan. Atomic parameters are given in Table 1, bond distances and angles in Table 2.* Fig. 1 shows the molecular structure and numbering scheme.

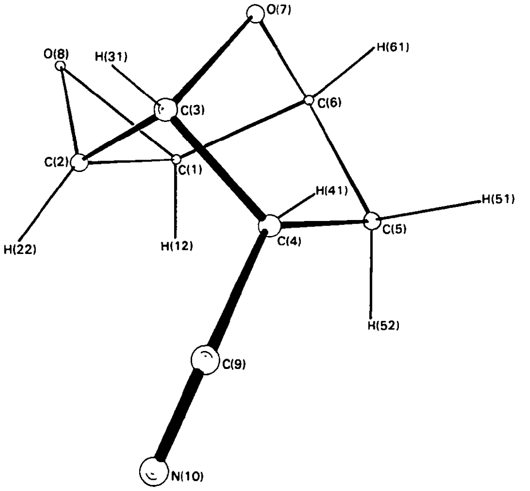

Fig. 1. The molecular structure with the numbering scheme.

Related literature. The present research was initiated to confirm the postulated *endo* position of the cyano group in the first compound isolated by Marfisi, Cossu & Aycard (1981). The structure may be compared to those of 6-chloro-6-cyano-1,5-dimethyl-3,8-dioxatricyclo[3.2.1.0^{2,4}]octane (Cossu, Viani, Lapasset, Aycard, Marfisi & Bodot, 1982) and related cyano compounds (Viani, Cossu & Lapasset, 1981).

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* Lists of structure factors, torsion angles and shortest intermolecular contacts have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43229 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1986). C**42**, 1887–1889

Structure of 1,2,3-Triaminoguanidine (TAG)

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(*Received* 5 *December* 1985; *accepted* 28 *May* 1986)

Abstract. CH_8N_6, $M_r = 104{\cdot}2$, monoclinic, $P2_1/c$, $a = 7{\cdot}460$ (3), $b = 10{\cdot}274$ (2), $c = 6{\cdot}343$ (3) Å, $\beta = 110{\cdot}80$ (2)°, $V = 454{\cdot}5$ Å^3, $Z = 4$, $D_x = 1{\cdot}52$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54184 Å, $\mu = 10{\cdot}1$ cm^{-1}, $F(000) = 224$, $T = 168$ (1) K, final $R = 0{\cdot}031$ for 771 unique observed reflections. One C—N distance [1·292 (1) Å] in the TAG molecule is significantly short; all other bond distances fall within the accepted ranges for C—N and

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N—N single-bond lengths. The structure consists of sheets of TAG molecules oriented in the direction of the *b* axis and held together by molecular forces and hydrogen bonds. Closest non-hydrogen-bonded intermolecular N···N contact is 3·220 (1) Å. Closest hydrogen-bonded intermolecular N···N contact is 2·967 (1) Å.

Experimental. A colorless plate-like crystal synthesized at this laboratory (0·15 × 0·05 × 0·30mm) was mounted on its long axis parallel to the φ axis of the goniometer. An Enraf–Nonius CAD-4 computer-controlled κ-axis diffractometer equipped with a graphite-crystal incident-beam monochromator was used. Lattice parameters were obtained using 23 reflections in the range $9 < \theta < 74°$. Intensity data for 1659 reflections (932 unique, $R_{\rm int} = 0{\cdot}037$), $h = 0$ to 9, $k = 0$ to 12, $l = -7$ to 7 (upper limit 150° 2θ), were collected with the ω–θ scan technique and were corrected for Lorentz and polarization effects. Three standard reflections were monitored with less than 1% intensity variation. Systematic absences: $0k0$, $k = 2n + 1$; $h0l$, $l = 2n + 1$. No absorption correction was made. A secondary-extinction correction was applied (Zachariasen, 1963); the final coefficient refined to $1{\cdot}70 \times 10^{-5}$ (absolute units). Structure solved by *MULTAN* (Germain, Main & Woolfson, 1971) and refined with Enraf–Nonius *SDP* (Frenz, 1978). H atoms located by difference Fourier synthesis. Non-H atoms were refined anisotropically and H atoms refined isotropically. Function minimized: $\sum w(|F_o| - |F_c|)^2$; $w = 4F_o^2/\sigma^2(F_o)^2$. Scattering factors from Cromer & Waber (1974), anomalous dispersion included (Ibers & Hamilton, 1964) and f' and f'' values from Cromer (1974). Refinement of 97 parameters using 771 reflections ($I > 3\sigma$) converged with a largest parameter shift of 0·62 times its e.s.d.; $R = 0{\cdot}031$, $wR = 0{\cdot}044$, $S = 1{\cdot}3$. Final difference Fourier synthesis maximum peak 0·25 e Å^{-3} with an e.s.d. of 0·05. Table 1* gives the atomic parameters and Table 2 the interatomic distances and angles. Fig. 1 shows the molecule and atom-numbering scheme; Fig. 2 shows packing in the unit cell.

Table 1. *Atom coordinates and isotropic temperature factors and their e.s.d.'s*

$$B_{\rm eq} = \tfrac{1}{4}\textstyle\sum_i\sum_j B_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}/B_{\rm iso}$(Å^2)
C	0·2343 (1)	0·0361 (1)	0·1937 (2)	0·97 (2)
N(1)	0·2102 (1)	0·13278 (9)	0·0561 (1)	1·10 (2)
N(2)	0·3015 (1)	0·1115 (1)	−0·1083 (1)	1·20 (2)
N(3)	0·3294 (1)	−0·0761 (1)	0·1797 (2)	1·23 (2)
N(4)	0·3656 (1)	−0·1682 (1)	0·3580 (2)	1·78 (2)
N(5)	0·1583 (1)	0·0416 (1)	0·3629 (1)	1·11 (2)
N(6)	−0·0024 (1)	0·12554 (9)	0·3318 (1)	1·17 (2)
H(1)	0·273 (2)	0·188 (1)	−0·195 (2)	2·2 (3)
H(2)	0·236 (2)	0·039 (2)	−0·199 (2)	2·3 (3)
H(3)	0·433 (2)	−0·067 (2)	0·120 (3)	3·1 (4)
H(4)	0·351 (2)	−0·247 (2)	0·295 (3)	3·4 (4)
H(5)	0·478 (3)	−0·161 (2)	0·448 (3)	3·4 (4)
H(6)	0·141 (2)	−0·035 (1)	0·409 (2)	1·5 (3)
H(7)	0·042 (2)	0·203 (1)	0·396 (2)	1·8 (3)
H(8)	−0·056 (2)	0·143 (2)	0·182 (2)	2·4 (4)

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

C(1)—N(1)	1·292 (1)	N(1)—N(2)	1·451 (1)
C(1)—N(3)	1·373 (1)	N(3)—N(4)	1·425 (1)
C(1)—N(5)	1·381 (1)	N(5)—N(6)	1·432 (1)
N(1)—C(1)—N(3)	123·57 (9)	C(1)—N(1)—N(2)	112·43 (9)
N(1)—C(1)—N(5)	119·8 (1)	C(1)—N(3)—N(4)	117·58 (9)
N(3)—C(1)—N(5)	116·65 (9)	C(1)—N(5)—N(6)	118·14 (9)

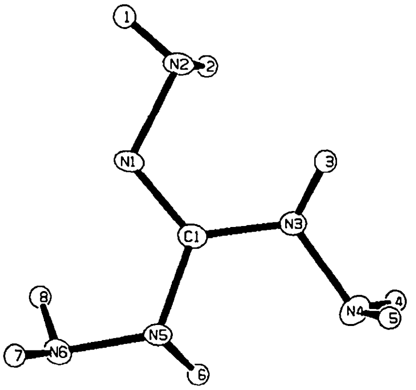

Fig. 1. Triaminoguanidine molecule. *ORTEP* plot (Johnson, 1976) with thermal ellipsoids scaled to enclose 50% probability.

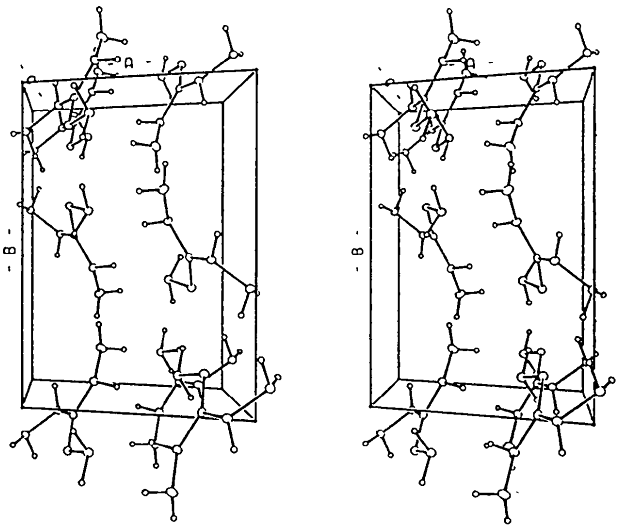

Fig. 2. Stereographic pair showing triaminoguanidine structure as viewed down the *c* axis. *ORTEP* plot with thermal ellipsoids scaled to enclose 20% probability.

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* Lists of structure factors, anisotropic thermal parameters, interatomic hydrogen distances and angles, and hydrogen-bonding details have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43110 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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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Acta Cryst. (1986). C**42**, 1889–1890

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}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ 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.

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

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

	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	

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}, $0 \leq h \leq 12$, $0 \leq k \leq 12$, $-16 \leq l \leq 16$. 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

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