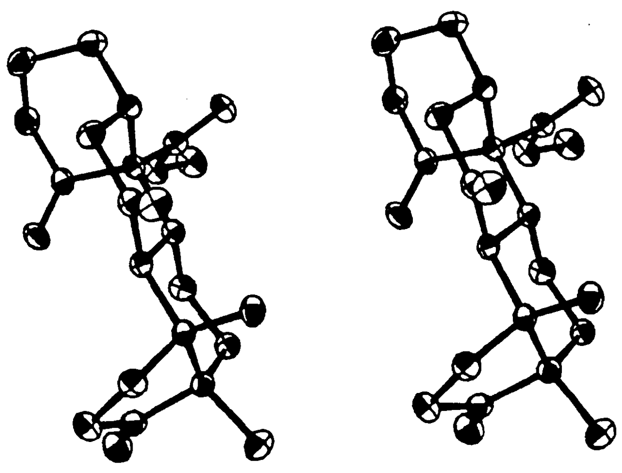

Fig. 2. *ORTEP* stereoview (Johnson, 1976).

Rings *C* and *D* are very similar to their homologues in compound (3) (Douglas *et al.*, 1987) leading to the conclusion that the main influence of the 1β,4β-methano bridge present in compound (3) is to force a boat conformation on rings *A* and *B*.

The chair conformation of ring *B* contributes to the folding of the molecule with rings *A* and *D* facing towards each other. The resulting overall conformation of the steroid (Fig. 3) is rather similar to that of compound (3). An intramolecular hydrogen bond between the C(7)—O(2) carbonyl group and the O(3)—H contributes to the stabilization of the molecular structure and particularly the chair conformation: d[O(2)···O(3)] = 2·703 (1), d[O(2)···HO(3)] = 1·98 (1), d[O(3)—HO(3)] = 0·86 (1) Å, $\angle$[O(2)···HO(3)—O(3)] = 141 (1°).

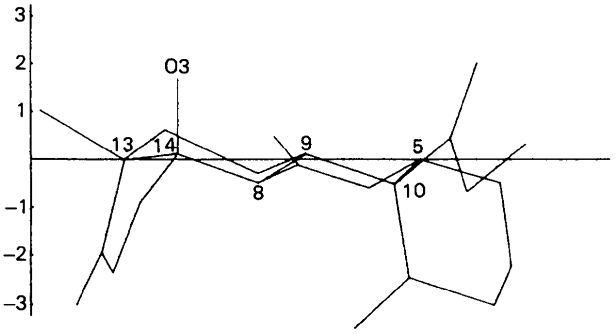

Fig. 3. Overall conformation of the steroid, viewed parallel to the least-squares mean plane through rings *B* and *C* (scale in Å).

The distance between these two functions is much greater in compound (3) where ring *B* is in a boat conformation (Douglas *et al.*, 1987). No abnormally short intermolecular contacts were observed in the crystal packing.

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Structure of 2-Cyclohexylamino-4,6-dimethoxy-1,3,5-triazine

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Abstract. $C_{11}H_{18}N_4O_2$, $M_r = 238·4$, triclinic, $P\bar{1}$, $a = 6·894$ (4), $b = 8·138$ (1), $c = 12·201$ (6) Å, $\alpha = 108·67$ (2), $\beta = 90·42$ (3), $\gamma = 105·41$ (1)°, $V = 621·97$ Å^3, $Z = 2$, $D_x = 1·272$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0·8$ mm^{-1}, $F(000) = 256$. The structure was solved by direct methods and refined to $R = 0·069$ for 2225 observed intensities. Delocalization of the *s*-triazine π electrons ranges over adjacent O and N atoms resulting in the formation of a planar 2-amino-4,6-dimethoxy-1,3,5-triazine system with stacking of triazine rings and perpendicular orientation of the cyclohexane mean plane in relation to the triazine plane.

Introduction. Derivatives of alkylamino-1,3,5-triazines have been used as herbicides. It has been suggested that a possible mechanism by which triazines are absorbed by soil mineral matter is the formation of coordination complexes with exchangeable cations of clay minerals (Hance, 1969).

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Recently, 2-chloro-4,6-disubstituted-*s*-triazines have been shown to be extremely efficient in the activation of carboxylic groups. A high yield in the synthesis of esters, amides, peptides and carboxylic acid anhydrides results even in the case of sterically hindered substrates (Kamiński, 1984*a*,*b*). The activation of carboxylic groups proceeds *via* the highly reactive ester. Greater reactivity of triazine esters compared with their phenyl analogues may result either from a different charge distribution in the ring or from different electronic and geometrical factors in the substituents, or both (Główka, Iwanicka & Kamiński, 1989). To explain the phenomenon a project on the structure–activity relationships of triazine derivatives was started and the present work is part of these studies.

Experimental. The compound was crystallized from methanol by slow evaporation of the solvent. A single crystal of dimensions 0·36 × 0·44 × 0·48 mm was used for data collection and accurate cell determination on a CAD-4 diffractometer with graphite-monochromatized Mo $K\alpha$ radiation. Unit-cell parameters were obtained from a least-squares refinement of 25 reflections in the θ range 9 to 16°. 2564 independent intensities [2225 considered observed with $I > 2\sigma(I)$] were measured with the $\omega/2\theta$ scan technique ($\theta_{\max} = 25°$, $-1 \leq h \leq 8$, $-9 \leq k \leq 9$, $-14 \leq l \leq 14$). Three standards monitored during data collection did not show significant change in intensity. No correction for absorption was applied.

The structure was solved by direct methods (*SHELXS*86, Sheldrick, 1986) and refined by full-matrix least squares on F (*SHELX*76, Sheldrick, 1976) with anisotropic temperature factors for non-H and isotropic ones for H atoms. The largest Δ/σ in the final cycle was 0·02. The final weighting scheme $w^{-1} = \sigma^2(F) + 0{\cdot}0074\,(F)^2$ was used; $R = 0{\cdot}069$, $wR = 0{\cdot}091$ and $S = 1{\cdot}15$. The final difference Fourier map showed no peaks above 0·4 e Å^{-3}. All calculations were performed on an Amstrad 1512 microcomputer. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974).

Discussion. The final atomic coordinates and equivalent isotropic temperature factors are presented in Table 1,* while bond distances and angles are given in Table 2. The atom-numbering system and a general view of the molecule are shown in Fig. 1.

Table 1. *Final positional and equivalent isotropic temperature parameters for non-*H *atoms with e.s.d.'s in parentheses.*

$$B_{eq} = \tfrac{4}{3}(a^{*2}B_{11} + \cdots + b^*c^*B_{23}\cos\alpha^*).$$

	x	y	z	B_{eq}(Å^2)
N(1)	0·3527 (3)	0·6854 (2)	0·6583 (1)	3·74 (5)
C(2)	0·4052 (3)	0·8051 (3)	0·6013 (2)	3·58 (6)
N(3)	0·3732 (3)	0·7633 (2)	0·4846 (1)	3·74 (6)
C(4)	0·2884 (3)	0·5899 (3)	0·4285 (2)	3·51 (6)
O(4)	0·2565 (3)	0·5485 (2)	0·3128 (1)	4·69 (5)
N(5)	0·2321 (3)	0·4569 (2)	0·4734 (1)	3·75 (5)
C(6)	0·2695 (3)	0·5184 (3)	0·5887 (2)	3·49 (6)
O(6)	0·2114 (3)	0·3855 (2)	0·6473 (1)	4·43 (5)
N(7)	0·4975 (4)	0·9778 (2)	0·6631 (2)	4·45 (6)
C(7)	0·5552 (4)	1·0475 (3)	0·7881 (2)	4·03 (7)
C(8)	0·4469 (4)	1·1851 (3)	0·8497 (2)	4·63 (7)
C(9)	0·5116 (5)	1·2607 (3)	0·9807 (2)	5·18 (9)
C(10)	0·7387 (5)	1·3352 (3)	1·0082 (2)	5·74 (9)
C(11)	0·8459 (5)	1·1973 (3)	0·9463 (2)	5·45 (9)
C(12)	0·7830 (4)	1·1248 (3)	0·8153 (2)	4·50 (8)
C(13)	0·1329 (5)	0·2125 (3)	0·5790 (3)	5·84 (10)
C(14)	0·1711 (5)	0·3652 (4)	0·2447 (2)	5·10 (9)

Table 2. *Bond lengths* (Å), *valency angles* (°) *and selected torsion angles* (°) *for non-*H *atoms*

N(1)—C(2)	1·347 (3)	C(2)—N(1)—C(6)	113·2 (2)
N(1)—C(6)	1·318 (2)	C(4)—N(5)—C(6)	111·7 (2)
N(5)—C(4)	1·335 (3)	C(4)—O(4)—C(14)	118·1 (2)
N(5)—C(6)	1·331 (3)	C(4)—N(3)—C(2)	113·9 (2)
O(4)—C(4)	1·344 (3)	C(6)—O(6)—C(13)	116·5 (2)
O(4)—C(14)	1·412 (3)	O(4)—C(4)—N(3)	113·9 (2)
N(3)—C(4)	1·319 (2)	N(5)—C(4)—N(3)	127·7 (2)
N(3)—C(2)	1·355 (3)	N(5)—C(4)—O(4)	118·5 (2)
O(6)—C(6)	1·453 (3)	C(2)—N(7)—C(7)	125·2 (2)
O(6)—C(13)	1·344 (3)	N(3)—C(2)—N(7)	116·9 (2)
N(7)—C(2)	1·337 (2)	N(1)—C(2)—N(7)	118·3 (2)
N(7)—C(7)	1·457 (3)	N(1)—C(2)—N(3)	124·7 (2)
C(7)—C(8)	1·513 (4)	N(5)—C(6)—O(6)	116·5 (2)
C(7)—C(12)	1·519 (4)	N(1)—C(6)—O(6)	114·7 (2)
C(8)—C(9)	1·532 (3)	N(1)—C(6)—N(5)	128·7 (2)
C(9)—C(10)	1·513 (5)	N(7)—C(7)—C(12)	111·2 (2)
C(12)—C(11)	1·530 (4)	N(7)—C(7)—C(8)	111·3 (2)
C(11)—C(10)	1·511 (3)	C(8)—C(7)—C(12)	111·4 (2)
		C(7)—C(8)—C(9)	111·0 (2)
C(14)—O(4)—C(4)—N(5)	−2·1 (4)	C(8)—C(9)—C(10)	112·4 (2)
C(13)—O(6)—C(6)—N(5)	2·5 (4)	C(7)—C(12)—C(11)	111·7 (2)
C(7)—N(7)—C(2)—N(1)	2·9 (4)	C(12)—C(11)—C(10)	110·9 (2)
C(2)—N(7)—C(7)—C(12)	117·2 (3)	C(9)—C(10)—C(11)	111·7 (2)

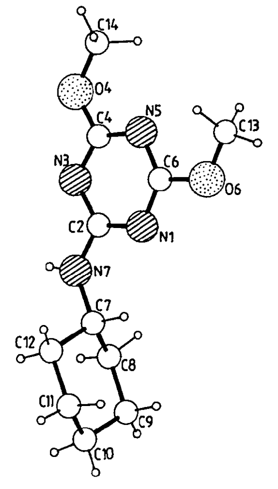

Fig. 1. General view of the molecule with numbering system.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52034 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The N—C bonds in the triazine ring range from 1·31 to 1·36 Å and average endocyclic angles at the N and C atoms are 112·3 and 127·8°, respectively. Similar differentation of bonds and angles in the *s*-triazine ring according to the type and arrangement of substituents is characteristic of the *s*-triazine system and has been observed previously (Graham, Akrigg & Sheldrick, 1977, 1978*a*,*b*; Reck & Jankowsky, 1981; Reck, Bannier, Just & Goldhahn, 1985). The exocyclic bond distance C(2)—N(7) = 1·337 (2) Å is in the same range as the C—N distances in the triazine ring. This indicates a wide delocalization of π electrons. Therefore, C(7) deviates from the ring plane by only 0·16 Å, and the torsion angle N(1)—C(2)—N(7)—C(7) is 2·9 (4) Å. Similar conjugation of lone pairs of electrons at O atoms of the methoxy groups with ring π electrons is hinted at by the N(5)—C(4)—O(4)—C(14) and N(5)—C(6)—O(6)—C(13) torsion angles of −2·1 (4) and 2·6 (4)°, respectively.

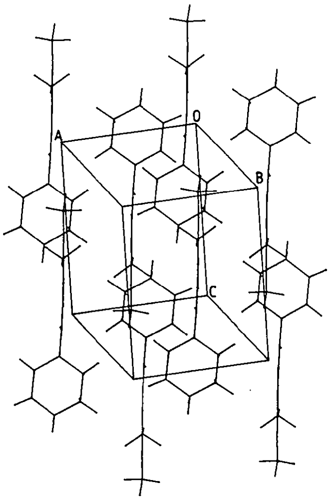

Fig. 2. The crystal packing.

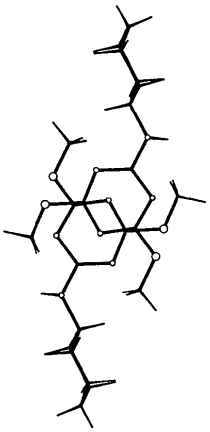

Fig. 3. The stacking of triazine systems in the crystal.

The only suspicious result of this study is the O(6)-atom position, which is evidenced by (*a*) C(6)—O(6) and O(6)—C(13) bond lengths of 1·453 (3) and 1·344 (3) Å, respectively, compared with 1·32 and 1·45 Å observed for other methoxy groups joined to the triazine system (Graham, Akrigg & Sheldrick, 1977, 1978*a*,*b*; Główka, Iwanicka & Kamiński, 1989); and (*b*) by an additional electron density peak of 0·39 e Å^{-3} located at 0·23 Å from the final O(6) position. Attempts to shift O(6) to a more 'accurate' position gave (after refinement) coordinates close to those listed in Table 1. The separation of possible disordered O(6)-atom positions failed.

The packing of 2-cyclohexylamino-4,6-dimethoxy-1,3,5-triazine in the crystal is shown in Fig. 2. The planar 2-amino-4,6-dimethoxy-1,3,5-triazine fragments form molecular layers interrupted by cyclohexane rings oriented perpendicularly to the layers. There is a stacking of triazine systems (Fig. 3) similar to that of uracil (Steward & Jensen, 1967) with a distance of $a/2$ = 3·447 Å between the parallel triazine rings. Perpendicular orientation of the triazine and the mean cyclohexane planes (Fig. 2) results in a short intramolecular contact between an axial H(7) atom and an N(1) atom of 2· 32 (2) Å.

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