Discussion. Final atomic positions and equivalent isotropic thermal parameters are given in Table 1.* An *ORTEP* (Johnson, 1965) drawing of the molecule with the numbering of atoms is shown in Fig. 1. Bond lengths and angles are given in Table 2.

The deviations of each atom in the triazole ring from the mean plane are very small, and the three bonds of N(1) are almost coplanar. From the results above, it is suggested that the triazole ring has aromaticity and the hybridization of the N(1) atom is of the sp^2 type.

The dihedral angle between the mean plane of the naphthalene ring and that of the triazole ring is 56·8 (2)°.

As the triazole ring is asymmetric about the C(1)–N(1) axis, it is interesting to know which side of the triazole ring is near to the C(9)–C(10) axis. The torsion angle C(9)–C(1)–N(1)–N(2), −58·8 (6)°, shows that N(2) is much closer to the C(9)–C(10) axis than the C(2)–C(3) axis.

The angle C(1)–C(9)–C(8), 123·7 (5)°, is distinctly small compared with that of (II), 129·0° (Nagawa *et al.*, 1986). This is because the steric overcrowding of (I) is less than that of (II).

The packing of the molecules in the crystal is shown in Fig. 2. The crystal structure is stabilized mainly by van der Waals forces; the shortest intermolecular distance is 3·506 (6) Å for C(2)(x, y, z)···N(2)($\frac{1}{2}+x$, y, $\frac{1}{2}-z$).

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, and details of least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43315 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

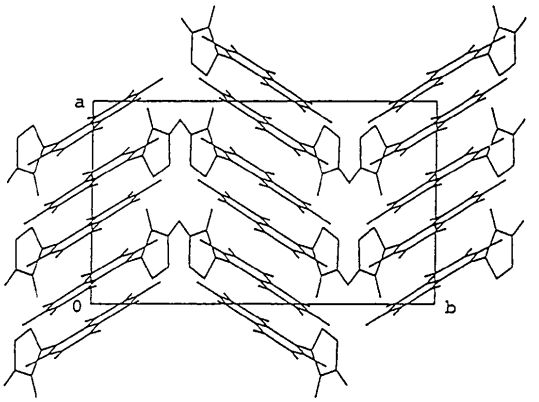

Fig. 2. Packing of molecules in the unit cell. (Positive c axis is taken downward.)

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4,6-Dimethoxy-1,3,5-triazin-2(1*H*)-one

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Abstract. $C_5H_7N_3O_3$, $M_r = 157·13$, orthorhombic, $Pca2_1$, $a = 12·027$ (3), $b = 14·579$ (3), $c = 7·776$ (2) Å, $V = 1363·5$ (5) Å^3, $Z = 8$, $D_x = 1·530$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0·14$ mm^{-1}, $F(000) = 656$, $T = 294$ K. Final $R = 0·034$ for 1184 observed [$I \geq 2\sigma(I)$] reflections. The two independent molecules of the asymmetric unit form dimers by means of two N–H···O(keto) hydrogen

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bonds with N···O distances of 2·822 (3) and 2·791 (3) Å. Bond lengths and angles in the two molecules agree within a 4σ limit. The 1,3,5-triazin-2(1*H*)-one system in one molecule is planar within 3σ whereas the deviations in the other molecule reach up to 30σ.

Introduction. Surprisingly few X-ray structures of triazinones and none of 1,3,5-triazin-2(1*H*)-one(s) are known, though their derivatives possess a remarkable herbicidal activity. The aza analogues of nucleosides and nucleotides comprising a triazinone ring have attracted much more attention owing to their anti-tumor properties. So far the crystal structures of 6-azauridine (Schwalbe & Saenger, 1973), 6-azauridine-5′-phosphate (Saenger & Suck, 1973) and 6-azacytidine (Singh & Hodgson, 1974) have been determined, all belonging to the 1,2,4-triazinone family.

The crystals of 4,6-dimethoxy-1,3,5-triazin-2(1*H*)-one (I) were obtained during a crystallization of a 2-*tert*-butoxy-4,6-dimethoxy-1,3,5-triazine from acetone after hydrolysis of the initial compound.

Experimental. White plates from acetone, 0·12 × 0·28 × 0·39 mm; Enraf–Nonius CAD-4 diffractometer, Mo $K\alpha$, graphite monochromator, lattice parameters from 25 reflections ($9 \le \theta \le 12°$). Data collection: 1588 independent reflections measured ($h_{max} = 15$, $k_{max} = 18$, $l_{max} = 9$ with $2\theta \le 54°$), three standard reflections monitored every 2 h, no significant intensity variation during data collection, 1186 observed with $I_o \ge 2\sigma(I_o)$, Lp correction, absorption not applied, space group $Pca2_1$ (No. 29); direct methods (*MULTAN*; Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1981), anisotropic full-matrix, H (from ΔF synthesis) isotropic, based on F; final cycle 254 parameters, $(\Delta/\sigma)_{max} = 0{\cdot}05$; $R = 0{\cdot}034$, $wR = 0{\cdot}041$, $S = 1{\cdot}21$, $w^{-1} = \sigma^2(I_o) + 0{\cdot}05|F_o|^2$; final ΔF has $\rho_{max} = 0{\cdot}145$ e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Programs used: *PARST* (Nardelli, 1983), CAD-4 *SDP* (Frenz, 1978) and *MULTAN*81 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1981). The final atomic parameters are listed in Table 1.*

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43330 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates and isotropic or equivalent isotropic thermal parameters* (Å^2)

$B_{eq} = \frac{4}{3}\sum_i\sum_j B_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	*y*	*z*	B_{eq}/B_{iso}
Molecule *A*				
O(1)	0·2384 (2)	0·3976 (1)	0·6522 (3)	3·53 (4)
O(2)	0·5943 (2)	0·3669 (1)	0·4622	4·10 (5)
O(3)	0·3446 (2)	0·1462 (1)	0·3575 (3)	3·38 (4)
N(1)	0·4654 (2)	0·2587 (1)	0·4032 (4)	2·91 (4)
N(3)	0·4180 (2)	0·3913 (1)	0·5588 (4)	2·95 (5)
N(5)	0·2858 (2)	0·2708 (1)	0·5127 (4)	3·16 (5)
C(1)	0·2600 (3)	0·4895 (2)	0·7156 (5)	3·73 (6)
C(2)	0·4969 (2)	0·3415 (2)	0·4761 (4)	2·88 (5)
C(3)	0·2358 (3)	0·1061 (2)	0·3832 (6)	4·69 (7)
C(4)	0·3199 (2)	0·3534 (2)	0·5714 (4)	2·78 (5)
C(6)	0·3617 (2)	0·2273 (2)	0·4280 (4)	2·68 (5)
H(1)	0·517 (3)	0·221 (2)	0·353 (5)	4·5 (7)
H(11)	0·323 (3)	0·488 (2)	0·786 (5)	5·5 (8)
H(12)	0·270 (3)	0·531 (2)	0·625 (6)	6·0 (8)
H(13)	0·187 (3)	0·507 (2)	0·759 (5)	5·6 (8)
H(31)	0·237 (2)	0·049 (1)	0·310 (4)	2·8 (6)
H(32)	0·209 (4)	0·107 (3)	0·518 (8)	9 (1)
H(33)	0·176 (4)	0·147 (2)	0·334 (7)	8 (1)
Molecule *B*				
O(1)	1·0018 (2)	0·0943 (1)	0·1733 (3)	3·17 (4)
O(2)	0·6339 (1)	0·1592 (1)	0·2329 (4)	3·99 (4)
O(3)	0·8894 (2)	0·3458 (1)	0·4615 (3)	3·57 (4)
N(1)	0·7644 (2)	0·2528 (1)	0·3443 (4)	3·09 (4)
N(3)	0·8149 (2)	0·1187 (1)	0·1955 (3)	3·00 (5)
N(5)	0·9529 (2)	0·2192 (1)	0·3162 (4)	2·85 (5)
C(1)	0·9780 (2)	0·0133 (2)	0·0732 (5)	3·83 (7)
C(2)	0·7327 (2)	0·1750 (2)	0·2564 (4)	2·92 (5)
C(3)	1·0046 (3)	0·3710 (2)	0·4973 (5)	3·86 (6)
C(4)	0·9171 (2)	0·1447 (2)	0·2282 (4)	2·57 (5)
C(6)	0·8736 (2)	0·2708 (2)	0·3718 (4)	2·68 (5)
H(1)	0·716 (2)	0·287 (2)	0·389 (4)	3·8 (7)
H(11)	0·941 (2)	0·031 (2)	−0·025 (4)	4·1 (7)
H(12)	1·051 (3)	−0·017 (2)	0·030 (5)	5·1 (8)
H(13)	0·924 (3)	−0·031 (2)	0·141 (5)	5·2 (8)
H(31)	1·002 (3)	0·419 (2)	0·581 (6)	6·0 (9)
H(32)	1·033 (3)	0·316 (2)	0·558 (6)	6·1 (9)
H(33)	1·041 (3)	0·396 (2)	0·391 (7)	7 (1)

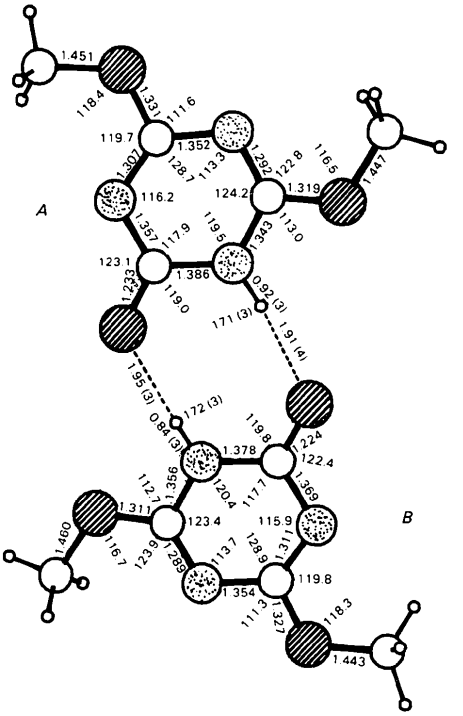

Fig. 1. A view of the dimer showing bond lengths and angles. The standard deviations (not shown) are 0·003–0·004 Å for distances and 0·2–0·3° for angles.

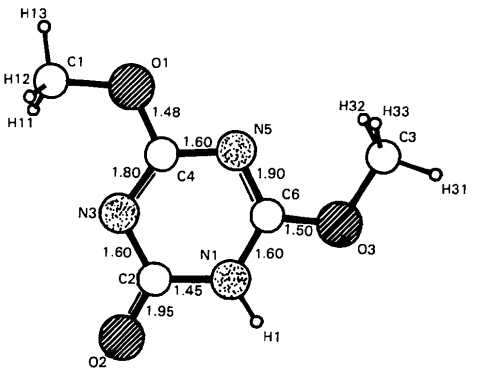

Fig. 2. Numbering of atoms and bond orders in the conjugated system.

Discussion. A view of the two independent molecules forming a dimer, together with bond lengths and angles for the non-hydrogen atoms, is shown in Fig. 1. Almost the whole molecule forms a conjugated system. The *p* atomic orbitals at the O(methoxy) and N(1) atoms overlap with π systems of the double C=O and C=N bonds, as evidenced by (i) shortening of O(1)–C(4), O(3)–C(6), N(1)–C(6) and N(1)–C(2) bonds to 1·33, 1·32, 1·35 and 1·38 Å, respectively, and (ii) coplanarity of methoxy groups with the triazine ring. All four independent methoxy groups are in a *syn* orientation towards the neighbouring 'most double' bond of the ring with the torsional angles N=C–O–Me less than 3·5°. There are significant differences among the C–N bond orders in the ring (Fig. 2) varying from 1·4 for N(1)–C(2) to 1·9 for N(5)–C(6), assuming single- and double-bond lengths of 1·47 and 1·27 Å, respectively (Pauling, 1960).

The main difference between the two molecules of (I) is in deviations of atoms from the least-squares ring plane. The deviations are up to 30σ [$\Delta C(2) = 0{\cdot}032$, $\Delta O(2) = 0{\cdot}103$, $\sigma_{mean} = 0{\cdot}003$ Å] in molecule *A* and 3σ in molecule *B*. The interplanar angle between rings *A* and *B* is 18·1 (1)°.

The bond lengths and angles in both independent molecules agree within 4σ limits.

This work is part of research project RPII.10.

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(±)-2-(4-Methoxyflavan-3-yl)-7-methoxyisoflav-3-ene*†

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Abstract. $C_{32}H_{28}O_4$, $M_r = 476{\cdot}6$, monoclinic, $P2_1/n$, $a = 12{\cdot}044$ (3), $b = 9{\cdot}517$ (5), $c = 21{\cdot}630$ (5) Å, $\beta = 91{\cdot}26$ (2)°, $U = 2479$ Å^3, $Z = 4$, $D_x = 1{\cdot}28$ g cm^{-3}, λ(Mo $K\alpha_1$) = 0·70926 Å, $\mu = 0{\cdot}8$ cm^{-1}, $F(000) = 1008$, $T = 293$ K, $R = 0{\cdot}045$ for 1399 observed reflections. The product from the condensation of 7-methoxyisoflavylium perchlorate with 3-(*o*-hydroxyphenyl)-1-(*p*-methoxyphenyl)propene is determined to be (±)-2-(4-methoxyflavan-3-yl)-7-methoxyisoflav-3-

* The Chemistry of the Insoluble Red Woods. 17. Part 16: Afonya, Epelle, Osman & Whalley (1985).

† Systematic name: 2-(2,3-dihydro-2-*p*-methoxyphenyl-4*H*-1-benzopyran-3-yl)-7-methoxy-3-phenyl-2*H*-1-benzopyran.

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