Table 1. *Atom coordinates and temperature factors* ($\mathring{A}^2$) *for* (1) *and* (2)

	x	y	z	U*
(1)				
N(1)	0·1507 (1)	0·3182 (1)	0·1029 (1)	0·054 (1)
C(2)	0·1967 (1)	0·4299 (2)	0·1390 (1)	0·046 (1)
N(3)	0·2815 (1)	0·5076 (2)	0·1109 (1)	0·050 (1)
C(4)	0·2590 (1)	0·6038 (2)	0·0591 (1)	0·048 (1)
S(5)	0·1187 (1)	0·6514 (1)	0·0232 (1)	0·057 (1)
C(6)	0·1306 (2)	0·7947 (2)	−0·0427 (1)	0·082 (1)
N(7)	0·1686 (1)	0·4661 (1)	0·2103 (1)	0·049 (1)
C(8)	0·0933 (2)	0·3781 (2)	0·2516 (1)	0·060 (1)
C(9)	0·2045 (1)	0·6001 (2)	0·2472 (1)	0·054 (1)
C(10)	0·1845 (2)	0·2767 (2)	0·0350 (1)	0·062 (1)
N(11)	0·2060 (2)	0·2284 (2)	−0·0231 (1)	0·093 (1)
S(12)	0·3681 (1)	0·6949 (1)	0·0220 (1)	0·071 (1)
C(13)	0·4915 (2)	0·6233 (3)	0·0814 (1)	0·086 (1)
C(81)	−0·0231 (1)	0·4401 (2)	0·2524 (1)	0·050 (1)
C(82)	−0·0853 (2)	0·4924 (2)	0·1839 (1)	0·062 (1)
C(83)	−0·1945 (2)	0·5426 (2)	0·1840 (1)	0·072 (1)
C(84)	−0·2426 (2)	0·5409 (2)	0·2535 (2)	0·078 (1)
C(85)	−0·1812 (2)	0·4913 (2)	0·3225 (1)	0·075 (1)
C(86)	−0·0726 (2)	0·4410 (2)	0·3220 (1)	0·062 (1)
C(91)	0·3232 (1)	0·6041 (2)	0·2918 (1)	0·052 (1)
C(92)	0·3920 (2)	0·7155 (2)	0·2829 (1)	0·075 (1)
C(93)	0·4983 (2)	0·7281 (3)	0·3273 (2)	0·097 (1)
C(94)	0·5363 (2)	0·6283 (3)	0·3804 (2)	0·099 (1)
C(95)	0·4697 (2)	0·5171 (3)	0·3900 (2)	0·110 (1)
C(96)	0·3629 (2)	0·5038 (2)	0·3462 (1)	0·084 (1)
(2)				
N(1)	1·0338 (1)	0·9095 (1)	0·1943 (1)	0·035 (1)
C(2)	1·0973 (2)	1·0073 (1)	0·2726 (2)	0·032 (1)
N(3)	1·2397 (1)	1·0017 (1)	0·3485 (1)	0·037 (1)
C(4)	1·3187 (2)	0·9033 (1)	0·3642 (2)	0·031 (1)
S(5)	1·2944 (1)	0·7727 (1)	0·4471 (1)	0·041 (1)
C(6)	1·1507 (2)	0·8101 (2)	0·5082 (2)	0·052 (1)
N(7)	1·0274 (2)	1·1063 (1)	0·2809 (2)	0·044 (1)
N(8)	1·4345 (1)	0·9041 (1)	0·3296 (1)	0·033 (1)
C(9)	1·5464 (2)	0·8101 (2)	0·3603 (2)	0·044 (1)
C(10)	1·6593 (2)	0·8587 (2)	0·3061 (2)	0·057 (1)
C(11)	1·5795 (2)	0·9510 (2)	0·1986 (2)	0·057 (1)
C(12)	1·4679 (2)	1·0031 (1)	0·2517 (2)	0·041 (1)
N(13)	0·8985 (1)	0·9182 (1)	0·0975 (1)	0·036 (1)
O(14)	0·8396 (1)	0·8233 (1)	0·0444 (1)	0·054 (1)
O(15)	0·8326 (1)	1·0129 (1)	0·0562 (1)	0·055 (1)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

—NO₂ and especially a better electron donor —NC₄H₈, with the consequence that structures having a double bond between C(2) and N(3) and a single bond between N(3) and C(4) are enhanced relative to (1). The large out-of-plane twist about N(3)—C(4) in (2) is in the range found for other

Table 2. *Bond lengths* ($\mathring{A}$) *for* (1) *and* (2)

(1)			
N(1)—C(2)	1·315 (2)	N(1)—C(10)	1·327 (3)
C(2)—N(3)	1·385 (2)	C(2)—N(7)	1·340 (2)
N(3)—C(4)	1·275 (2)	C(4)—S(5)	1·752 (2)
C(4)—S(12)	1·745 (2)	S(5)—C(6)	1·788 (2)
N(7)—C(8)	1·471 (2)	N(7)—C(9)	1·467 (2)
C(8)—C(81)	1·505 (3)	C(9)—C(91)	1·505 (2)
C(10)—N(11)	1·145 (3)	S(12)—C(13)	1·796 (2)
C(81)—C(82)	1·381 (2)	C(81)—C(86)	1·382 (3)
C(82)—C(83)	1·382 (3)	C(83)—C(84)	1·372 (3)
C(84)—C(85)	1·376 (3)	C(85)—C(86)	1·375 (3)
C(91)—C(92)	1·365 (3)	C(91)—C(96)	1·370 (3)
C(92)—C(93)	1·383 (3)	C(93)—C(94)	1·348 (4)
C(94)—C(95)	1·350 (4)	C(95)—C(96)	1·384 (3)
(2)			
N(1)—C(2)	1·371 (2)	N(1)—N(13)	1·333 (2)
C(2)—N(3)	1·324 (2)	C(2)—N(7)	1·332 (2)
N(3)—C(4)	1·331 (2)	C(4)—S(5)	1·762 (2)
C(4)—N(8)	1·307 (2)	S(5)—C(6)	1·789 (3)
N(8)—C(9)	1·477 (2)	N(8)—C(12)	1·478 (2)
C(9)—C(10)	1·511 (3)	C(10)—C(11)	1·507 (3)
C(11)—C(12)	1·507 (3)	N(13)—O(14)	1·244 (2)
N(13)—O(15)	1·242 (2)		

sterically hindered push-pull systems (Gilardi, Flippen-Anderson & George, 1989).

H atoms H(7a) and H(7b) in (2) were refined with N···H and H···H distances constrained to 0·96 and 1·663 Å. The distance O(15)···H(7a) 1·987 (13) Å indicates a hydrogen bond, with bond angle at H(7a) 120·0 (8)°.

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Structures of 1,2,3-Triazine Derivatives

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Abstract. (I) 4-Methyl-6-phenyl-1,2,3-triazine, $C_{10}H_9N_3$, $M_r = 171·2$, monoclinic, $P2_1/c$, $a = 10·684$ (1), $b = 13·755$ (1), $c = 6·074$ (1) Å, $\beta = 103·28$ (1)°, $U = 868·8$ (2) Å³, $Z = 4$, $D_x = 1·309$ Mg m⁻³, $\mu = 0·667$ mm⁻¹, $F(000) = 360$, final $R = 0·055$ for 909 reflexions. (II) 4-Phenylcyclohexa-

Table 1. *Details of data collection and structure refinement*

	(I)	(II)	(III)	(IV)	(V)
Data collection					
Crystal size (mm)	0·50 × 0·45 × 0·25	0·40 × 0·30 × 0·55	0·55 × 0·30 × 0·55	0·30 × 0·20 × 0·40	0·45 × 0·55 × 0·15
Cell-parameter determination: No. of reflexions; θ range (°)	20; 59–61	20; 58–60	20; 56–60	25; 53–56	20; 58–61
Scan speed (° min⁻¹)	16·0	16·0	16·0	8·0	16·0
Max. $(\sin\theta)/\lambda$ (Å⁻¹)	0·56	0·56	0·56	0·46	0·56
Range of h	−11–11	0–12	−13–13	0–10	−15–15
k	0–15	0–10	0–12	0–13	0–9
l	0–6	0–22	0–8	0–7	0–6
Standard reflexions: No.; interval; intensity variation (%)	3; 150; < 3·0	3; 150; < 3·0	3; 150; < 3·0	3; 150; < 3·0	3; 150; < 3·0
No. of reflexions	1549	1945	1792	702	1316
independent	1293	1633	1527	670	1083
$F > 3\sigma(F)$	909	1386	1341	623	955
Merging R for equivalent	0·036	—	0·031	—	0·038
reflexions	140	—	134	—	121
Systematic absences	$h0l$: $l \neq 2n$ $0k0$: $k \neq 2n$ $00l$: $l \neq 2n$	$0kl$: $l \neq 2n$ $h0l$: $h \neq 2n$ $hk0$: $k \neq 2n$ $h00$: $h \neq 2n$ $0k0$: $k \neq 2n$ $00l$: $l \neq 2n$	$h0l$: $h + l \neq 2n$ $h00$: $h \neq 2n$ $0k0$: $k \neq 2n$ $00l$: $l \neq 2n$	$h00$: $h \neq 2n$ $0k0$: $k \neq 2n$ $00l$: $l \neq 2n$	$h0l$: $h \neq 2n$ $h00$: $h \neq 2n$ $0k0$: $k \neq 2n$
Refinement					
R	0·055	0·047	0·050	0·057	0·058
wR	0·060	0·050	0·062	0·050	0·054
G^*	1·534	1·679	1·206	2·629	1·789
$(\Delta/\sigma)_{max}$	0·15	0·20	0·20	0·24	0·38
$\Delta\rho_{max}/\Delta\rho_{min}$ (e Å⁻³)	0·41/−0·22	0·40/−0·26	0·63/−0·32	0·68/−0·31	0·51/−0·40

$$* \; G = \Sigma w\{[|(|F_c|)^2 - (|F_c|)^2|]^2/(N_r - N_v)\}^{1/2}.$$

[d][1,2,3]triazine, $C_{13}H_{13}N_3$, $M_r = 211\cdot3$, orthorhombic, *Pcab*, $a = 11\cdot224\,(1)$, $b = 9\cdot817\,(2)$, $c = 19\cdot939\,(4)$ Å, $U = 2197\cdot1\,(3)$ Å³, $Z = 8$, $D_x = 1\cdot277$ Mg m⁻³, $\mu = 0\cdot629$ mm⁻¹, $F(000) = 896$, final $R = 0\cdot047$ for 1386 reflexions. (III) 4-Methyl-6-phenyl-1,2,3-triazine 2-oxide, $C_{10}H_9N_3O$, $M_r = 187\cdot2$, monoclinic, $P2_1/n$, $a = 11\cdot486\,(2)$, $b = 10\cdot897\,(1)$, $c = 7\cdot235\,(2)$ Å, $\beta = 100\cdot69\,(2)°$, $U = 889\cdot9\,(3)$ Å³, $Z = 4$, $D_x = 1\cdot397$ Mg m⁻³, $\mu = 0\cdot788$ mm⁻¹, $F(000) = 392$, final $R = 0\cdot050$ for 1341 reflexions. (IV) 4,6-Dimethyl-1,2,3-triazine 2-oxide, $C_5H_7N_3O$, $M_r = 125\cdot1$, orthorhombic, $P2_12_12_1$, $a = 8\cdot932\,(1)$, $b = 11\cdot743\,(1)$, $c = 6\cdot073\,(1)$ Å, $U = 637\cdot1\,(3)$ Å³, $Z = 4$, $D_x = 1\cdot305$ Mg m⁻³, $\mu = 0\cdot812$ mm⁻¹, $F(000) = 264$, final $R = 0\cdot057$ for 623 reflexions. (V) 4,5,6-Trimethyl-1,2,3-triazin-2-imine, $C_6H_{10}N_4$, $M_r = 138\cdot1$, monoclinic, $P2_1/a$, $a = 14\cdot211\,(1)$, $b = 8\cdot477\,(1)$, $c = 6\cdot190\,(1)$ Å, $\beta = 100\cdot79\,(1)°$, $U = 732\cdot5\,(1)$ Å³, $Z = 4$, $D_x = 1\cdot253$ Mg m⁻³, $\mu = 0\cdot687$ mm⁻¹, $F(000) = 296$, final $R = 0\cdot058$ for 955 reflexions. $\lambda(\text{Cu }K\alpha_1) = 1\cdot5405$ Å and $T = 293$ K for all five determinations. Of the N⸺N distances in the N(2)-substituted 1,2,3-triazines (III), (IV) and (V), the largest differences are observed for (V) (0·039 and 0·035 Å longer than those found in unsubstituted 1,2,3-triazine). Larger N(1)—N(2)—N(3) angles of 126·1 (1) (III), 126·3 (2) (IV) and 124·4 (3)° (V) than 122·3 (2) (I) and 121·8 (1)° (II) are observed. The bond distances in the N(2)-oxides (N⁺—O⁻) and N(2)-imine (N⁺—NH⁻) are 1·247 (2) (III), 1·251 (4) (IV) and 1·286 (5) Å (V), respectively. The torsion angles between the triazine rings and their phenyl rings are 17·1 (3) (I), 44·2 (3) (II) and 7·4 (3)° (III).

Introduction. 1,2,3-Triazines, one of the basic azabenzenes, which are the least studied class when compared with the other two possible triazine ring systems, have attracted considerable interest (Neunhoeffer, 1978). In the course of our work on the chemistry of 1,2,3-triazines, various derivatives have been synthesized including unsubstituted 1,2,3-triazine (Ohsawa, Arai, Ohnishi & Igeta, 1981; Ohsawa, Kaihoh, Itoh, Okada, Kawabata, Yamaguchi & Igeta, 1988). Five 1,2,3-triazine derivatives including an N(2)-imine (Ohsawa, Arai, Ohnishi, Itoh, Yamaguchi, Kaihoh, Kawabata & Igeta, 1988) and N(2)-oxides (Ohsawa, Arai, Ohnishi, Kaihoh, Yamaguchi, Igeta & Iitaka, 1986) were subjected to X-ray crystallographic analysis, in order to investigate structural properties of the 1,2,3-triazine ring system.
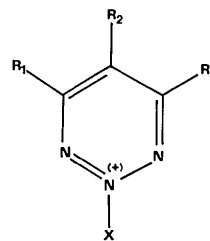
(I) $R_1 = \text{Me}$, $R_2 = \text{H}$, $R_3 = \text{Ph}$
(II) R_1–$R_2 = (\text{CH}_2)_4$, $R_3 = \text{Ph}$
(III) $R_1 = \text{Me}$, $R_2 = \text{H}$, $R_3 = \text{Ph}$, $X = \text{O}^-$
(IV) $R_1 = R_3 = \text{Me}$, $R_2 = \text{H}$, $X = \text{O}^-$
(V) $R_1 = R_2 = R_3 = \text{Me}$, $X = \text{NH}^-$

Experimental. Preparation and physical properties of (I), (III), (IV) and (V) are given by Ohsawa *et al.* (1981, 1986), Ohsawa, Arai *et al.* (1988) and Ohsawa,

Kaihoh *et al.* (1988). (II) was obtained by *N*-amination of the corresponding aminopyrazole and successive oxidation, using identical procedures as described in the above reports. Details of data collection and refinement are listed in Table 1. Intensity data were collected with a Rigaku AFC5 diffractometer; graphite-monochromated Cu $K\alpha_1$ radiation; θ–2θ scan method; $(1\cdot3 + 0\cdot41\tan\theta)°$ scan width; intensities were corrected for Lorentz and polarization factors, absorption correction was not applied. Structures were solved using program package *SAPI*85 (Yao, Zheng, Qian, Han, Gu & Fan, 1985) version of *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Refinement was carried out by the full-matrix least-squares method with anisotropic thermal parameters for non-H atoms; the function minimized was $\sum w[(|F_o|)^2 - (|F_c|)^2]^2$ with $w = 1/[\sigma^2(F_o) + 0\cdot02(F_o)^2]$, $\sigma(F_o)$ was determined from counting statistics; all H atoms were located from the difference maps and theoretical calculations, the initial thermal parameters were set at the equivalent isotropic thermal parameters of the bonded atoms. All calculations were performed using a PANAFACOM computer with the *RCRYSTAN* (Rigaku Corpora-

tion, 1985) X-ray analysis program system. Atomic scattering factors were those from *International Tables for X-ray Crystallography* (1974).

Discussion. Final atomic parameters for compounds (I)–(V) are listed in Table 2. Selected bond lengths and angles are listed in Table 3. Fig. 1 shows *ORTEP* drawings (Johnson, 1965) of molecules (I)–(V), Fig. 2 gives the crystal structures.* In (I), the bond lengths and angles of the triazine ring are consistent with those found in unsubstituted 1,2,3-triazine (Yamaguchi, Ohsawa, Arai, Ohnishi, Igeta & Iitaka, 1983). The N$\doteq$N and N$\doteq$C bond lengths are close to the respective lengths in 1,2,3-triazine [1·313 (4) and 1·322 (4) Å for N$\doteq$N, 1·339 (5) and 1·344 (5) Å for N$\doteq$C]. The consistency in these bond lengths is also found in (II). However, differences in the N$\doteq$N lengths are found in (III), (IV) and (V).
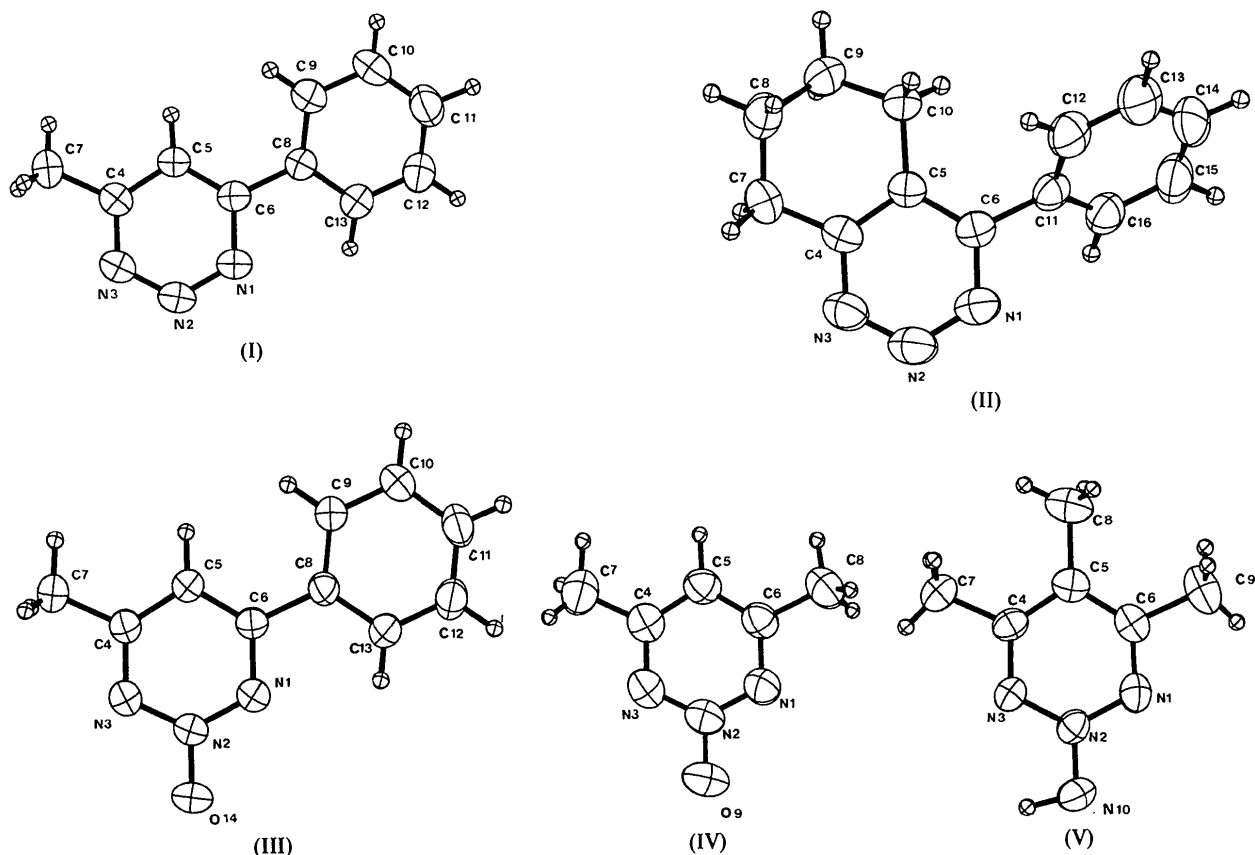
(I)

(II)

(III)   (IV)   (V)

Fig. 1. *ORTEP* drawings of compounds (I) to (V).

The largest lengthening, by 0·039 and 0·035 Å from that found in the N-free 1,2,3-triazines, is observed in (V). It can be seen that the N(1)—N(2)—N(3) angles for (III), (IV) and (V) are large compared with those for (I) and (II). N(2)—N(3)—C(4) and C(6)—N(1)—N(2) angles have the opposite tendency in compliance with the change in the N(1)—N(2)—N(3) angle. These differences between the N-free and N-oxide or N-imine compounds possibly point to an effect of back donation by the negative oxygen or

nitrogen system as observed in pyridine N-oxides (*Comprehensive Heterocyclic Chemistry*, 1984). The N(2)-oxides (N⁺—O⁻) and N(2)-imine (N⁺—NH⁻) bond distances indicate that the contribution of the double-bond character to these bonds is greater than that found in pyridine N-oxides [1·33 and 1·37 Å (Ulku, Huddle & Morrow, 1971)]. The triazine rings are planar within experimental error for each compound, indicating extensive electron delocalization in the rings. The torsion angles between the triazine and
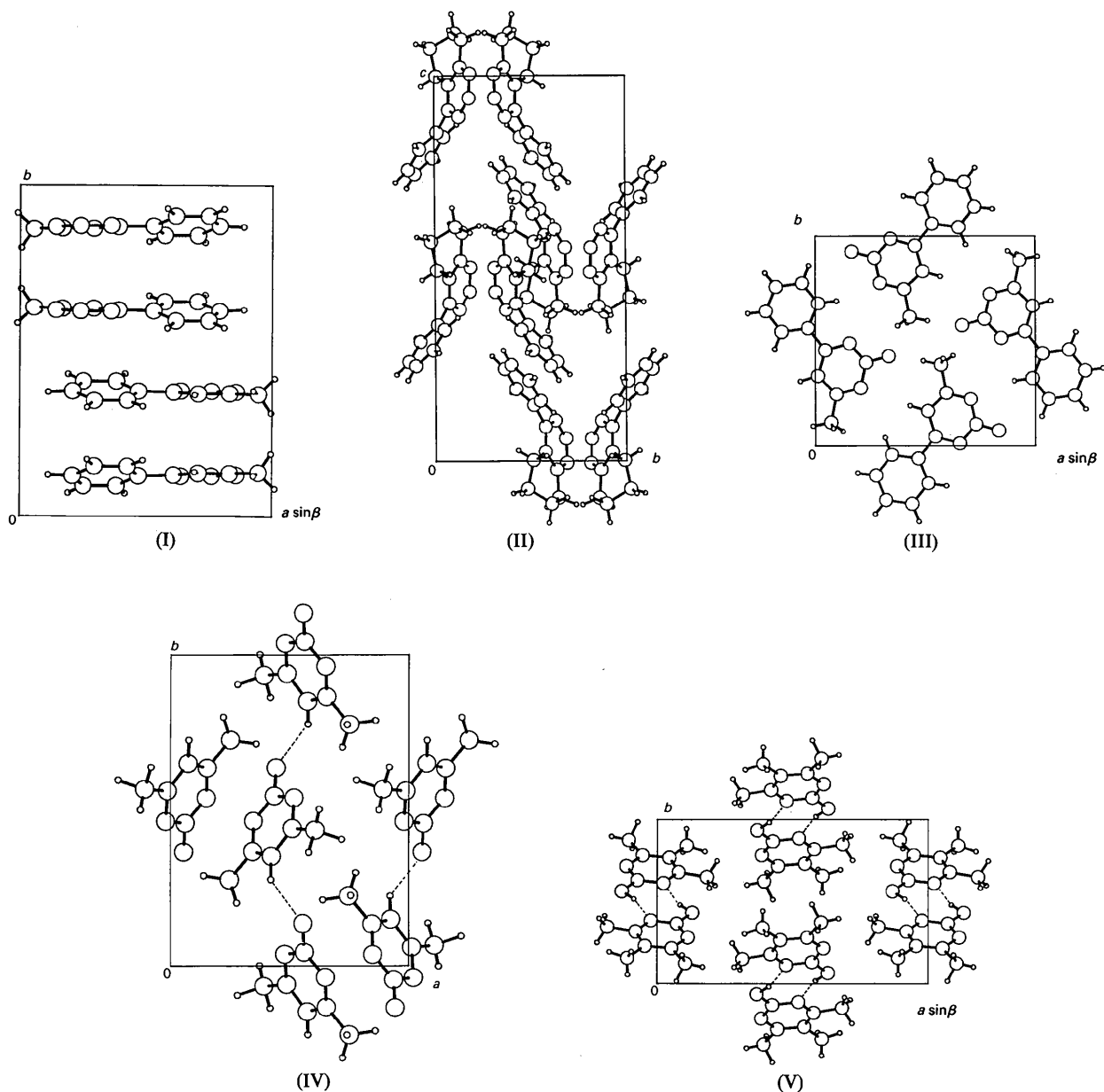

Fig. 2. Projections of the structures of compounds (I) to (V).

Table 2. *Atomic coordinates and equivalent isotropic thermal parameters* ($\mathring{A}^2$)

	x	y	z	B_{eq}†
(I)				
N(1)	0·3613 (2)	0·6204 (1)	0·8219 (3)	5·13 (8)
N(2)	0·2402 (2)	0·6209 (2)	0·8369 (4)	5·98 (9)
N(3)	0·1432 (2)	0·6238 (2)	0·6558 (4)	5·50 (8)
C(4)	0·1686 (2)	0·6284 (2)	0·4505 (4)	4·40 (8)
C(5)	0·2930 (2)	0·6292 (2)	0·4248 (4)	4·23 (8)
C(6)	0·3902 (2)	0·6240 (2)	0·6168 (4)	3·77 (7)
C(7)	0·0542 (3)	0·6311 (4)	0·2561 (6)	6·53 (14)
C(8)	0·5290 (2)	0·6215 (2)	0·6197 (4)	3·72 (7)
C(9)	0·5734 (2)	0·6496 (2)	0·4311 (5)	4·61 (9)
C(10)	0·7037 (2)	0·6503 (2)	0·4393 (6)	5·41 (10)
C(11)	0·7907 (3)	0·6215 (2)	0·6318 (6)	5·40 (10)
C(12)	0·7476 (3)	0·5912 (2)	0·8174 (6)	5·34 (10)
C(13)	0·6173 (2)	0·5912 (2)	0·8120 (5)	4·63 (9)
(II)				
N(1)	0·5572 (1)	0·3719 (1)	0·3948 (1)	4·43 (5)
N(2)	0·4894 (1)	0·3171 (1)	0·4421 (1)	5·09 (5)
N(3)	0·5236 (1)	0·3127 (1)	0·5057 (1)	4·59 (5)
C(4)	0·6297 (1)	0·3654 (1)	0·5233 (1)	3·55 (5)
C(5)	0·7044 (1)	0·4256 (1)	0·4770 (1)	3·21 (4)
C(6)	0·6640 (1)	0·4249 (1)	0·4110 (1)	3·42 (5)
C(7)	0·6584 (2)	0·3570 (2)	0·5965 (1)	4·39 (6)
C(8)	0·7871 (2)	0·3930 (2)	0·6115 (1)	4·81 (7)
C(9)	0·8224 (2)	0·5199 (2)	0·5730 (1)	4·77 (7)
C(10)	0·8204 (2)	0·4896 (2)	0·4984 (1)	4·18 (6)
C(11)	0·7307 (1)	0·4856 (2)	0·3542 (1)	3·71 (5)
C(12)	0·8488 (2)	0·4511 (2)	0·3425 (1)	5·02 (7)
C(13)	0·9095 (2)	0·5104 (3)	0·2898 (1)	6·30 (9)
C(14)	0·8546 (2)	0·6035 (3)	0·2490 (1)	6·37 (9)
C(15)	0·7370 (2)	0·6377 (2)	0·2597 (1)	5·58 (8)
C(16)	0·6755 (2)	0·5781 (2)	0·3119 (1)	4·36 (6)
(III)				
N(1)	0·6561 (1)	0·0127 (1)	0·3679 (2)	3·74 (4)
N(2)	0·7307 (1)	0·1029 (1)	0·4329 (2)	3·82 (4)
N(3)	0·7059 (1)	0·2231 (1)	0·4263 (2)	3·83 (4)
C(4)	0·5955 (1)	0·2530 (1)	0·3445 (2)	3·45 (4)
C(5)	0·5116 (1)	0·1665 (1)	0·2716 (2)	3·44 (4)
C(6)	0·5459 (1)	0·0450 (1)	0·2864 (2)	3·06 (4)
C(7)	0·5710 (2)	0·3870 (1)	0·3372 (4)	4·84 (6)
C(8)	0·4676 (1)	−0·0599 (1)	0·2166 (2)	3·14 (4)
C(9)	0·3474 (1)	−0·0424 (1)	0·1483 (2)	4·08 (5)
C(10)	0·2751 (1)	−0·1411 (2)	0·0858 (3)	4·68 (5)
C(11)	0·3211 (2)	−0·2584 (1)	0·0911 (2)	4·43 (5)
C(12)	0·4400 (2)	−0·2764 (1)	0·1553 (2)	4·46 (5)
C(13)	0·5134 (1)	−0·1780 (1)	0·2183 (2)	3·87 (4)
O(14)	0·8333 (1)	0·0729 (1)	0·5082 (2)	5·62 (4)
(IV)				
N(1)	0·6507 (3)	−0·0369 (2)	0·0547 (6)	5·05 (7)
N(2)	0·5626 (3)	0·0442 (2)	−0·0254 (6)	5·16 (8)
N(3)	0·4803 (3)	0·0379 (2)	−0·2081 (5)	4·90 (7)
C(4)	0·4881 (3)	−0·0601 (2)	−0·3187 (6)	4·48 (8)
C(5)	0·5751 (4)	−0·1494 (2)	−0·2495 (6)	4·55 (8)
C(6)	0·6547 (4)	−0·1343 (2)	−0·0595 (6)	4·50 (8)
C(7)	0·3924 (6)	−0·0657 (5)	−0·5190 (8)	6·62 (13)
C(8)	0·7520 (6)	−0·2244 (4)	0·0374 (11)	6·90 (16)
O(9)	0·5561 (4)	0·1357 (2)	0·0799 (6)	7·62 (10)
(V)				
N(1)	0·8863 (2)	0·7174 (3)	0·0115 (4)	3·99 (9)
N(2)	0·9273 (1)	0·6323 (3)	0·1890 (4)	3·46 (8)
N(3)	1·0232 (1)	0·6134 (3)	0·2556 (4)	3·52 (8)
C(4)	1·0798 (2)	0·6809 (4)	0·1333 (5)	3·42 (9)
C(5)	1·0447 (2)	0·7684 (4)	−0·0543 (5)	3·61 (10)
C(6)	0·9463 (2)	0·7829 (4)	−0·1043 (5)	3·74 (10)
C(7)	1·1840 (2)	0·6511 (6)	0·2143 (9)	5·13 (14)
C(8)	1·1101 (4)	0·8421 (7)	−0·1909 (9)	5·81 (17)
C(9)	0·8948 (4)	0·8757 (6)	−0·2983 (8)	5·69 (16)

$$† B_{eq} = \tfrac{4}{3}\Sigma_i\Sigma_j B_{ij}\mathbf{a}_i{}^*\mathbf{a}_j{}^*\mathbf{a}_i.\mathbf{a}_j.$$

Table 3. *Bond lengths* ($\mathring{A}$) *and angles* (°) *in the triazine rings*

	(I)	(II)	(III)	(IV)	(V)
N(1)—N(2)	1·317 (4)	1·329 (3)	1·330 (2)	1·327 (4)	1·352 (4)
N(2)—N(3)	1·327 (3)	1·324 (3)	1·340 (2)	1·334 (5)	1·357 (4)
N(3)—C(4)	1·337 (3)	1·345 (3)	1·337 (2)	1·334 (5)	1·333 (5)
C(4)—C(5)	1·373 (4)	1·382 (3)	1·380 (2)	1·370 (5)	1·389 (5)
C(5)—C(6)	1·374 (3)	1·391 (3)	1·380 (3)	1·368 (6)	1·380 (5)
C(6)—N(1)	1·351 (4)	1·345 (3)	1·341 (2)	1·338 (5)	1·334 (5)
N(1)—N(2)—N(3)	122·3 (2)	121·8 (1)	126·1 (1)	126·3 (2)	124·4 (3)
N(2)—N(3)—C(4)	119·1 (2)	119·4 (1)	115·6 (1)	116·0 (2)	117·0 (2)
N(3)—C(4)—C(5)	121·0 (2)	121·9 (2)	122·6 (1)	122·2 (3)	122·9 (3)
C(4)—C(5)—C(6)	117·7 (2)	115·6 (1)	117·1 (1)	117·1 (3)	115·1 (3)
C(5)—C(6)—N(1)	119·7 (2)	121·1 (1)	121·2 (1)	122·3 (3)	124·4 (3)
C(6)—N(1)—N(2)	119·9 (2)	119·9 (1)	117·0 (1)	115·9 (3)	115·8 (2)

no intermolecular distances are significantly shorter than the sums of the respective van der Waals radii. Short contacts of $C(5)\cdots O(9)(-x+1,\ y-\tfrac{1}{2},\ -z-\tfrac{1}{2})$ 3·432 (5) and $H(5)\cdots O(9)$ 2·49 (4) $\mathring{A}$ in (IV) suggest attractive C—H⋯O interactions (Robin & Kennard, 1982). The hydrogen bond $N(3)\cdots N(10)(-x+2,\ -y+1,\ -z+1)$ was observed in (V) $[N(3)\cdots N(10)$ 3·275 (4), $N(3)\cdots H(10)$ 2·32 (2) $\mathring{A}]$.

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phenyl rings in (I), (II) and (III) are 17·1 (3), 44·2 (3) and 7·4 (3)°, respectively. The largest value, in (II), is ascribed to the steric hindrance resulting from the C(5)-substituted methylene moiety. In the crystals of (I), (II) and (III) there are no hydrogen bonds and