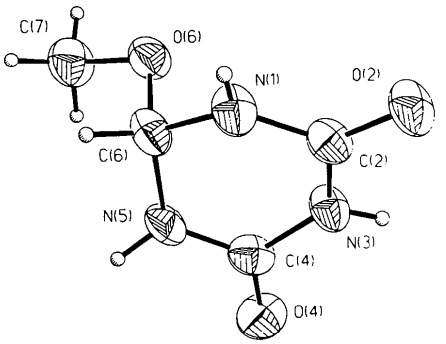

Fig. 1. Thermal-ellipsoid plot of 5-aza-6-methoxyuracil with ellipsoids drawn at 50% probability level.

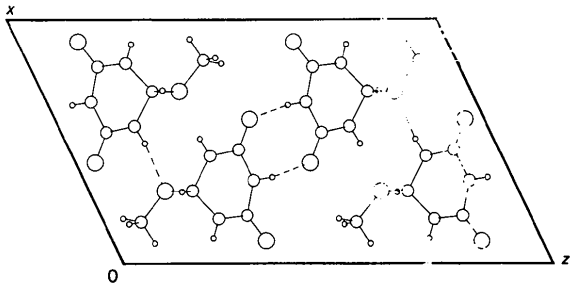

Fig. 2. Unit-cell contents viewed down **b**.

used *SHELXTL* (Sheldrick, 1980). $\sum w(|F_o| - |F_c|)^2$ minimized where $w = 1/[\sigma^2(|F_o|) + g(F_o)^2]$, $g = 0{\cdot}00030$. 106 parameters refined: atom coordinates, anisotropic temperature factors for all non-H atoms, isotropic temperature factors for H atoms, methyl-H atoms included using riding model, C—H = 0·96 Å, H—C—H = 109·5°, $U(\mathrm{H}) = 1{\cdot}2U_{eq}(\mathrm{C})$. $(\Delta/\sigma)_{max} = 0{\cdot}009$, $R = 0{\cdot}050$, $wR = 0{\cdot}058$, $S = 1{\cdot}884$. Final difference Fourier excursions 0·32 and −0·22 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).* Atom numbering for Tables 1 and 2, which give atom coordinates, bond distances and bond angles, follows that shown in Fig. 1; Fig. 2 shows the packing and hydrogen bonding.

Related literature. Structures with related ring connectivity include cyanuric acid (Verschoor & Keulen, 1971) and 2,4,6-triamino-*s*-triazine (Cromer, Larson & Stewart, 1976).

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* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43399 (8 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. (1987). C**43**, 364–366

Bis(*m*-nitrobenzyl) Ether

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Abstract. $C_{14}H_{12}N_2O_5$, $M_r = 288{\cdot}26$, triclinic, $P\bar{1}$, $a = 7{\cdot}644$ (2), $b = 8{\cdot}378$ (2), $c = 12{\cdot}331$ (3) Å, $\alpha = 71{\cdot}96$ (2), $\beta = 74{\cdot}66$ (2), $\gamma = 63{\cdot}83$ (2)°, $U = 666{\cdot}3$ Å^3, $Z = 2$, $D_x = 1{\cdot}44$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 1{\cdot}0$ cm^{-1}, $F(000) = 300$, $T = 293$ K, $R = 0{\cdot}049$ for 1774 reflections. The two halves of the molecule differ in the torsion angles about the O—CH_2 bonds [163·3 (3), 174·9 (3)°] and about the C—Ar bonds [−35·4 (4), 146·9 (3)° for one ring, −7·6 (4), 172·2 (3)° for the other].

Experimental. Yellow prism, 0·6 × 0·4 × 0·15 mm, by diffusion of petrol into CH_2Cl_2 solution. Stoe–Siemens four-circle diffractometer, monochromated Mo $K\alpha$ radiation, profile-fitting mode (Clegg, 1981). 2326 reflections, $2\theta_{max}$ 50°, $-h \pm k \pm l$, 2321 unique, 1774 with

0108-2701/87/020364-03$01.50

Table 1. *Atom coordinates* ($\times 10^4$) *and isotropic temperature factors* (Å$^2 \times 10^3$)

	x	y	z	U_{eq}*
O(1)	3220 (2)	8031 (2)	7235 (1)	63 (1)
C(1)	2712 (3)	9134 (3)	6159 (1)	54 (1)
C(11)	4081 (3)	8211 (2)	5215 (1)	44 (1)
C(12)	5729 (3)	6613 (2)	5433 (1)	42 (1)
C(13)	6940 (3)	5833 (2)	4527 (1)	43 (1)
C(14)	6582 (3)	6576 (3)	3406 (2)	57 (1)
C(15)	4939 (3)	8151 (3)	3197 (2)	64 (1)
C(16)	3699 (3)	8964 (3)	4083 (2)	58 (1)
N(13)	8665 (2)	4122 (2)	4775 (2)	55 (1)
O(31)	9028 (2)	3508 (2)	5762 (1)	71 (1)
O(32)	9652 (2)	3382 (2)	3978 (1)	83 (1)
C(1′)	2096 (4)	8889 (3)	8154 (2)	73 (1)
C(11′)	2262 (3)	7502 (3)	9277 (2)	55 (1)
C(12′)	2396 (3)	5779 (3)	9334 (1)	52 (1)
C(13′)	2419 (3)	4574 (2)	10384 (1)	50 (1)
C(14′)	2327 (3)	5005 (3)	11391 (2)	67 (1)
C(15′)	2227 (3)	6707 (3)	11331 (2)	74 (1)
C(16′)	2214 (3)	7937 (3)	10286 (2)	64 (1)
N(3′)	2559 (3)	2752 (2)	10422 (1)	64 (1)
O(31′)	2774 (3)	2330 (2)	9523 (1)	88 (1)
O(32′)	2429 (3)	1730 (2)	11358 (1)	100 (1)

* Equivalent isotropic U calculated from anisotropic U.

Table 2. *Bond lengths* (Å), *bond angles* (°) *and torsion angles* (°)

C(1)–O(1)	1·401 (3)	C(1)–C(11)	1·500 (4)
C(11)–C(12)	1·386 (3)	C(11)–C(16)	1·392 (4)
C(12)–C(13)	1·380 (3)	C(13)–C(14)	1·374 (4)
C(13)–N(13)	1·470 (3)	C(14)–C(15)	1·373 (4)
C(15)–C(16)	1·378 (4)	N(13)–O(31)	1·220 (4)
N(13)–O(32)	1·221 (3)	C(1′)–O(1)	1·409 (3)
C(1′)–C(11′)	1·500 (4)	C(11′)–C(12′)	1·382 (4)
C(11′)–C(16′)	1·388 (5)	C(12′)–C(13′)	1·372 (3)
C(13′)–C(14′)	1·373 (4)	C(13′)–N(3′)	1·469 (4)
C(14′)–C(15′)	1·374 (5)	C(15′)–C(16′)	1·378 (4)
N(3′)–O(31′)	1·215 (4)	N(3′)–O(32′)	1·216 (3)

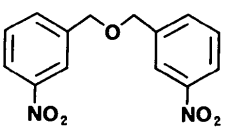
C(1)–O(1)–C(1′)	112·8 (2)	O(1)–C(1)–C(11)	110·0 (2)
C(1)–C(11)–C(12)	121·9 (3)	C(1)–C(11)–C(16)	119·6 (2)
C(12)–C(11)–C(16)	118·5 (3)	C(11)–C(12)–C(13)	119·2 (3)
C(12)–C(13)–C(14)	122·7 (2)	C(12)–C(13)–N(13)	118·6 (3)
C(14)–C(13)–N(13)	118·7 (3)	C(13)–C(14)–C(15)	117·8 (3)
C(14)–C(15)–C(16)	120·9 (3)	C(11)–C(16)–C(15)	120·9 (3)
C(13)–N(13)–O(31)	118·5 (3)	C(13)–N(13)–O(32)	118·0 (3)
O(31)–N(13)–O(32)	123·5 (2)	O(1)–C(1′)–C(11′)	110·2 (3)
C(1′)–C(11′)–C(12′)	120·5 (3)	C(1′)–C(11′)–C(16′)	120·9 (3)
C(12′)–C(11′)–C(16′)	118·6 (3)	C(11′)–C(12′)–C(13′)	119·3 (3)
C(12′)–C(13′)–C(14′)	122·6 (3)	C(12′)–C(13′)–N(3′)	118·2 (3)
C(14′)–C(13′)–N(3′)	119·2 (3)	C(13′)–C(14′)–C(15′)	118·1 (3)
C(14′)–C(15′)–C(16′)	120·4 (4)	C(11′)–C(16′)–C(15′)	121·0 (4)
C(13′)–N(3′)–O(31′)	119·1 (3)	C(13′)–N(3′)–O(32′)	118·4 (3)
O(31′)–N(3′)–O(32′)	122·5 (3)		

C(1′)–O(1)–C(1)–C(11)	174·9 (3)	C(1)–O(1)–C(1′)–C(11′)	163·3 (3)
O(1)–C(1)–C(11)–C(12)	−7·6 (4)	O(1)–C(1)–C(11)–C(16)	172·2 (3)
C(1)–C(11)–C(12)–C(13)	−179·6 (3)	C(16)–C(11)–C(12)–C(13)	0·5 (5)
C(1)–C(11)–C(16)–C(15)	179·6 (4)	C(12)–C(11)–C(16)–C(15)	−0·5 (5)
C(11)–C(12)–C(13)–C(14)	0·0 (5)	C(11)–C(12)–C(13)–N(13)	−179·0 (3)
C(12)–C(13)–C(14)–C(15)	−0·5 (5)	N(13)–C(13)–C(14)–C(15)	178·5 (3)
C(12)–C(13)–N(13)–O(31)	−4·2 (4)	C(12)–C(13)–N(13)–O(32)	175·3 (3)
C(14)–C(13)–N(13)–O(31)	176·8 (3)	C(14)–C(13)–N(13)–O(32)	−3·7 (4)
C(13)–C(14)–C(15)–C(16)	0·4 (5)	C(14)–C(15)–C(16)–C(11)	0·1 (6)
O(1)–C(1′)–C(11′)–C(12′)	−35·4 (4)	O(1)–C(1′)–C(11′)–C(16′)	146·9 (3)
C(1′)–C(11′)–C(12′)–C(13′)	−175·9 (3)	C(16′)–C(11′)–C(12′)–C(13′)	1·9 (4)
C(1′)–C(11′)–C(16′)–C(15′)	175·4 (3)	C(12′)–C(11′)–C(16′)–C(15′)	−2·3 (4)
C(11′)–C(12′)–C(13′)–C(14′)	−0·4 (4)	C(11′)–C(12′)–C(13′)–N(3′)	179·9 (3)
C(12′)–C(13′)–C(14′)–C(15′)	−0·6 (4)	N(3′)–C(13′)–C(14′)–C(15′)	179·0 (3)
C(12′)–C(13′)–N(3′)–O(31′)	4·6 (4)	C(12′)–C(13′)–N(3′)–O(32′)	−174·5 (3)
C(14′)–C(13′)–N(3′)–O(31′)	−175·1 (3)	C(14′)–C(13′)–N(3′)–O(32′)	5·8 (4)
C(13′)–C(14′)–C(15′)–C(16′)	0·2 (4)	C(14′)–C(15′)–C(16′)–C(11′)	1·3 (4)

$F > 4\sigma(F)$ used for all calculations (program system *SHELXTL*; Sheldrick, 1983). Index ranges after merging $|h| \le 8$, $|k| \le 9$, $|l| \le 14$. Three check reflections, no significant intensity variation. No absorption correction. Cell constants refined from $\pm 2\theta$ values of 42 reflections in the range 20–23°.

Structure solution by routine direct methods. Refinement on F to R 0·049, wR 0·054. All non-H atoms anisotropic; H atoms included using riding model with C–H 0·96 Å, H–C–H 109·5°, $U(\mathrm{H}) = 1{\cdot}2U_{eq}(\mathrm{C})$; weighting scheme $w^{-1} = \sigma^2(F) + 0{\cdot}0003F^2$; 190 parameters; $S = 1{\cdot}89$; max. Δ/σ 0·07; max. features in final $\Delta\rho$ map 0·16, −0·25 e Å^{-3}. Atomic scattering factors from *SHELXTL*. Final atomic coordinates are given in Table 1, and bond lengths and angles in Table 2.* Fig. 1 shows the atom-numbering scheme.

Related literature. The title compound (1) was prepared accidentally as part of a study of ethers and esters containing the 1-arylethyl group (Jones, Edwards & Kirby, 1986). See also Yufit, Yanovskii, Frolov & Struchkov (1983) for a *p*-nitrophenyl ether.



(1)

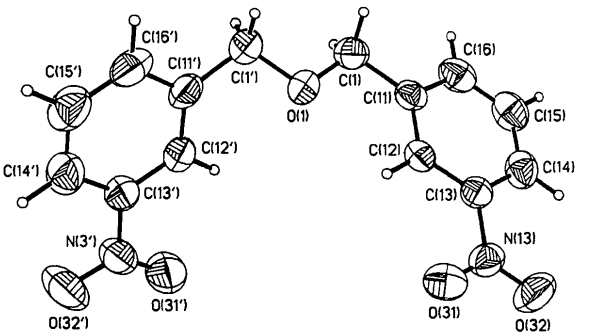


Fig. 1. Thermal ellipsoid plot of the molecule, showing the atom-numbering scheme.

* Lists of structure factors, H-atom coordinates, and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43067 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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1-(4-Nitrophenyl)ethyl *p*-Toluenesulfonate

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Abstract. $C_{15}H_{15}NO_5S$, $M_r = 321{\cdot}36$, orthorhombic, $Pca2_1$, $a = 13{\cdot}311\ (4)$, $b = 7{\cdot}643\ (2)$, $c = 15{\cdot}511\ (4)$ Å, $U = 1578$ Å^3, $Z = 4$, $D_x = 1{\cdot}35$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71069$ Å^3, $\mu = 2{\cdot}0$ cm^{-1}, $F(000) = 672$, $T = 293$ K, $R = 0{\cdot}063$ for 1859 reflections. The torsion angles of the Ar–S–O–C–Ar chain are 76·8 (5) and 117·4 (5)° about the S–O and O–C bonds, respectively.

Experimental. Colourless blocks from diffusion of petrol into CH_2Cl_2 solution. Fragment 0·4 × 0·4 × 0·35 mm cut from larger crystal. Stoe–Siemens four-circle diffractometer, monochromated Mo $K\alpha$ radiation, profile-fitting mode (Clegg, 1981). $2\theta_{max}$ 50°, 2958 reflections, octants $+h+k+l$ and $-h-k-l$. Three check reflections, no significant intensity variation. No absorption correction. 2766 unique reflections, R_{int} 0·020, index range $|h| \le 14$, $|k| \le 9$, $|l| \le 18$. 1859 reflections with $F > 4\sigma(F)$ used for all calculations (program system *SHELXTL*; Sheldrick, 1983). Cell constants refined from $\pm 2\theta$ values of 38 reflections in the range 20–23°.

Structure solution by random-start direct methods. Refinement on F to R 0·063, wR 0·059. All non-H

Table 1. *Atom coordinates* (× 10^4) *and isotropic temperature factors* (Å^2 × 10^3)

	x	*y*	*z*	U_{eq}*
S	5299 (1)	5108 (2)	5000	61 (1)
O(1)	5325 (3)	3374 (5)	4417 (2)	74 (2)
O(2)	4315 (3)	5619 (5)	5175 (2)	90 (2)
O(3)	5927 (3)	6213 (5)	4527 (3)	84 (2)
N(4)	2168 (5)	1068 (7)	1594 (4)	78 (2)
O(41)	2589 (4)	897 (7)	898 (3)	108 (2)
O(42)	1268 (4)	1031 (9)	1707 (3)	124 (2)
C(3)	4636 (4)	1951 (7)	4576 (3)	67 (2)
C(4)	5206 (5)	391 (8)	4835 (4)	93 (3)
C(11)	5895 (4)	4494 (6)	5974 (3)	52 (2)
C(12)	6902 (4)	4154 (7)	5971 (3)	62 (2)
C(13)	7362 (4)	3700 (7)	6738 (4)	71 (2)
C(14)	6834 (5)	3552 (7)	7505 (3)	64 (2)
C(15)	5835 (6)	3890 (7)	7465 (4)	73 (2)
C(16)	5330 (4)	4332 (7)	6716 (3)	64 (2)
C(17)	7357 (6)	3085 (9)	8327 (4)	96 (3)
C(21)	4010 (4)	1774 (6)	3794 (3)	51 (2)
C(22)	2984 (4)	2054 (6)	3819 (3)	59 (2)
C(23)	2395 (4)	1832 (7)	3122 (3)	59 (2)
C(24)	2820 (4)	1369 (7)	2354 (3)	53 (2)
C(25)	3823 (4)	1098 (7)	2272 (3)	64 (2)
C(26)	4421 (4)	1292 (7)	3004 (3)	67 (2)

* Equivalent isotropic U calculated from anisotropic U.

Table 2. *Bond lengths* (Å), *bond angles* (°) *and torsion angles* (°)

O(1)–S	1·604 (5)	O(2)–S	1·394 (5)
O(3)–S	1·396 (5)	N(4)–O(41)	1·223 (8)
N(4)–O(42)	1·210 (9)	C(3)–O(1)	1·444 (7)
C(3)–C(4)	1·469 (9)	C(11)–S	1·770 (6)
C(11)–C(12)	1·366 (8)	C(11)–C(16)	1·380 (8)
C(12)–C(13)	1·382 (9)	C(13)–C(14)	1·386 (9)
C(14)–C(15)	1·356 (11)	C(14)–C(17)	1·495 (10)
C(15)–C(16)	1·384 (9)	C(21)–C(3)	1·478 (8)
C(21)–C(22)	1·383 (9)	C(21)–C(26)	1·391 (8)
C(22)–C(23)	1·346 (9)	C(23)–C(24)	1·366 (8)
C(24)–N(4)	1·483 (9)	C(24)–C(25)	1·357 (9)
C(25)–C(26)	1·395 (8)		

O(1)–S–O(2)	111·2 (3)	O(1)–S–O(3)	101·0 (3)
O(2)–S–O(3)	119·7 (3)	O(1)–S–C(11)	104·6 (3)
O(2)–S–C(11)	109·2 (3)	O(3)–S–C(11)	109·9 (3)
S–O(1)–C(3)	120·8 (4)	O(41)–N(4)–O(42)	125·4 (7)
O(41)–N(4)–C(24)	116·7 (6)	O(42)–N(4)–C(24)	117·9 (6)
O(1)–C(3)–C(4)	109·3 (6)	O(1)–C(3)–C(21)	106·7 (5)
C(4)–C(3)–C(21)	116·2 (6)	S–C(11)–C(12)	119·1 (5)
S–C(11)–C(16)	119·5 (5)	C(12)–C(11)–C(16)	121·4 (6)
C(11)–C(12)–C(13)	118·6 (6)	C(12)–C(13)–C(14)	122·3 (6)
C(13)–C(14)–C(15)	116·2 (6)	C(13)–C(14)–C(17)	121·0 (7)
C(15)–C(14)–C(17)	122·8 (7)	C(14)–C(15)–C(16)	124·1 (7)
C(11)–C(16)–C(15)	117·2 (6)	C(3)–C(21)–C(22)	121·3 (6)
C(3)–C(21)–C(26)	121·7 (6)	C(22)–C(21)–C(26)	116·9 (6)
C(21)–C(22)–C(23)	122·3 (6)	C(22)–C(23)–C(24)	119·4 (6)
N(4)–C(24)–C(23)	119·4 (6)	N(4)–C(24)–C(25)	118·6 (6)
C(23)–C(24)–C(25)	122·0 (6)	C(24)–C(25)–C(26)	117·9 (6)
C(21)–C(26)–C(25)	121·4 (6)		

O(2)–S–O(1)–C(3)	−41·0 (5)	O(3)–S–O(1)–C(3)	−169·0 (5)
C(11)–S–O(1)–C(3)	76·8 (5)	O(1)–S–C(11)–C(12)	69·0 (5)
O(1)–S–C(11)–C(16)	−109·6 (5)	O(2)–S–C(11)–C(12)	−171·9 (5)
O(2)–S–C(11)–C(16)	9·5 (6)	O(3)–S–C(11)–C(12)	−38·8 (6)
O(3)–S–C(11)–C(16)	142·6 (5)	S–O(1)–C(3)–C(4)	−116·3 (5)
S–O(1)–C(3)–C(21)	117·4 (5)	O(41)–N(4)–C(24)–C(23)	170·1 (6)
O(41)–N(4)–C(24)–C(25)	−12·8 (9)	O(42)–N(4)–C(24)–C(23)	−9·0 (9)
O(42)–N(4)–C(24)–C(25)	168·1 (7)	O(1)–C(3)–C(21)–C(22)	−116·6 (6)
O(1)–C(3)–C(21)–C(26)	64·5 (7)	C(4)–C(3)–C(21)–C(22)	121·3 (7)
C(4)–C(3)–C(21)–C(26)	−57·6 (8)	S–C(11)–C(12)–C(13)	179·1 (5)
C(16)–C(11)–C(12)–C(13)	−2·3 (9)	S–C(11)–C(16)–C(15)	−178·5 (5)
C(12)–C(11)–C(16)–C(15)	2·9 (8)	C(11)–C(12)–C(13)–C(14)	1·1 (9)
C(12)–C(13)–C(14)–C(15)	−0·5 (9)	C(12)–C(13)–C(14)–C(17)	−179·0 (6)
C(13)–C(14)–C(15)–C(16)	1·2 (9)	C(17)–C(14)–C(15)–C(16)	179·7 (6)
C(14)–C(15)–C(16)–C(11)	−2·4 (9)	C(3)–C(21)–C(22)–C(23)	−177·3 (6)
C(26)–C(21)–C(22)–C(23)	1·7 (8)	C(3)–C(21)–C(26)–C(25)	178·9 (6)
C(22)–C(21)–C(26)–C(25)	−0·1 (8)	C(21)–C(22)–C(23)–C(24)	−2·2 (9)
C(22)–C(23)–C(24)–N(4)	178·0 (6)	C(22)–C(23)–C(24)–C(25)	1·0 (9)
N(4)–C(24)–C(25)–C(26)	−176·5 (6)	C(23)–C(24)–C(25)–C(26)	0·5 (9)

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