are given in Table 1,* and bond lengths and angles in Table 2. Fig. 1 shows the molecule and numbering scheme.

Related literature. For the preparation of the compound see Brüggemann (1983). For a recent structure of an indol derivative see Sawyer, Shariff & McLean (1985).

* Lists of structure factors, H-atom parameters and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42933 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2,3-Dimethoxy-1,4-butanedinitrile (I) and 2,3-Bis(piperidino)-1,4-butanedinitrile (II)

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Abstract. (I): $C_6H_8N_2O_2$, $M_r = 140{\cdot}14$, monoclinic, $P2_1/n$, $a = 9{\cdot}027$ (4), $b = 6{\cdot}756$ (3), $c = 6{\cdot}671$ (3) Å, $\beta = 107{\cdot}33$ (4)°, $V = 388{\cdot}4$ (3) Å^3, $Z = 2$, $D_x = 1{\cdot}20$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 1{\cdot}12$ cm^{-1}, $F(000) = 148$, $T = 291$ K, final $R = 0{\cdot}051$ for 404 observed reflections. (II): $C_{14}H_{22}N_4$, $M_r = 246{\cdot}36$, monoclinic, $C2/c$, $a = 23{\cdot}755$ (21), $b = 5{\cdot}571$ (6), $c = 11{\cdot}179$ (7) Å, $\beta = 99{\cdot}75$ (7)°, $V = 1458$ (2) Å^3, $Z = 4$, $D_x = 1{\cdot}12$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}75$ cm^{-1}, $F(000) = 536$, $T = 291$ K, final $R = 0{\cdot}052$ for 693 observed reflections. The two structures were examined to compare their geometry with that of purely captor substituted molecules. There are no unusual bond distances or angles. The central C—C bond is significantly shorter than that observed for 1,1,2,2-ethanetetracarbonitrile. The two molecules are strictly *meso*.

Experimental. Colourless parallelepipedal crystals from ethyl ether. Crystal dimensions: (I) 0·25 × 0·25 × 0·2 mm, (II) 0·2 × 0·18 × 0·3 mm. Syntex $P2_1$ diffractometer, graphite-monochromated Mo $K\alpha$ radiation. Unit cell from 15 reflections in range $5 < 2\theta < 20°$. Data collection: (I) 901 $hk\pm l$ unique, $0 \le h \le 11$, $0 \le k \le 8$, $-7 \le l \le 7$; max. $\sin\theta/\lambda = 0{\cdot}65$ Å^{-1}, (II) 2154 $h\pm k\pm l$ measured, 1080 unique ($R_{int} = 0{\cdot}031$), $0 \le h \le 26$, $0 \le k \le 6$, $-12 \le l \le 12$; max. $\sin\theta/\lambda = 0{\cdot}56$ Å^{-1}. 404 (I), 693 (II) reflections with $I \ge 2{\cdot}5\sigma(I)$ used in refinement. Standard reflections 221 (I), $\bar{4}2\bar{2}$ (II) checked every 50 reflections: no significant deviation. The two structures were solved by *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), and refined by full-matrix least squares with *SHELX*76 (Sheldrick, 1976) using F. H atoms from difference Fourier synthesis, included in refinement with isotropic common temperature factor. $w = 1/(\sigma^2 + gF^2)$, $g = 0{\cdot}0005$ (I), 0·0008 (II). $R = 0{\cdot}051$, $wR = 0{\cdot}051$ for 404 observed reflections (I); and $R = 0{\cdot}052$, $wR = 0{\cdot}054$ for 693 observed reflections (II). Final $(\Delta/\sigma)_{max} = 0{\cdot}24$ (I), 0·02 (II); $S = 2{\cdot}11$ (I), 1·51 (II). Max. and min. heights in final difference Fourier synthesis = 0·23 and −0·16 e Å^{-3} (I), 0·21 and

Table 1. *Atomic coordinates* (×10^4) *and equivalent isotropic temperature factors* (Å^2) *for* 2,3-*dimethoxy*-1,4-*butanedinitrile* (I)

$B_{eq} = \frac{8}{3}\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
C(1)	9418 (3)	4258 (5)	5169 (5)	3·52 (6)
C(2)	7886 (4)	4615 (5)	3582 (5)	4·18 (6)
N(3)	6710 (4)	4857 (5)	2414 (5)	6·56 (7)
O(4)	9308 (2)	4590 (4)	7197 (3)	4·84 (5)
C(5)	8509 (6)	3054 (8)	7918 (8)	6·59 (10)

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Table 2. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* ($Å^2$) *for* 2,3-*bis(piperidino)*-1,4-*butanedinitrile* (II)

$$B_{eq} = \tfrac{8}{3}\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j .$$

	x	y	z	B_{eq}
C(1)	2291 (1)	2620 (6)	4399 (3)	2·92 (6)
C(2)	2370 (1)	5012 (6)	3858 (3)	3·03 (6)
N(3)	2386 (1)	6824 (5)	3407 (3)	4·33 (6)
N(4)	1706 (1)	2192 (4)	4562 (2)	3·16 (5)
C(5)	1456 (2)	4081 (8)	5219 (4)	4·89 (8)
C(6)	879 (2)	3304 (11)	5474 (4)	6·53 (11)
C(7)	485 (2)	2686 (10)	4308 (5)	6·26 (10)
C(8)	763 (2)	842 (9)	3600 (6)	6·50 (11)
C(9)	1341 (2)	1678 (8)	3403 (4)	4·53 (8)

Table 3. *Interatomic distances* (Å) *and angles* (°)

	(I)	(II)
C(1)–C(2)	1·490 (5)	1·489 (4)
C(1)–C(1)*	1·517 (6)	1·535 (6)
C(2)–N(3)	1·126 (4)	1·132 (4)
C(1)–O(4)	1·403 (3)	—
O(4)–C(5)	1·426 (5)	—
C(1)–N(4)	—	1·450 (4)
N(4)–C(5)	—	1·466 (4)
N(4)–C(9)	—	1·460 (4)
Mean C–C in piperidino ring	—	1·509 (3)
C(1)*–C(1)–C(2)	108·9 (3)	109·0 (2)
C(1)*–C(1)–O(4)	106·8 (3)	—
C(1)*–C(1)–N(4)	—	111·6 (2)
C(2)–C(1)–O(4)	110·0 (3)	—
C(2)–C(1)–N(4)	—	112·8 (2)
C(1)–C(2)–N(3)	178·2 (3)	174·6 (3)
C(1)–O(4)–C(5)	113·4 (3)	—
C(1)–N(4)–C(5)	—	115·0 (3)
C(1)–N(4)–C(9)	—	111·1 (2)
C(5)–N(4)–C(9)	—	110·8 (3)
N(4)–C(5)–C(6)	—	110·3 (4)
N(4)–C(9)–C(8)	—	110·6 (4)
Mean C–C–C in piperidino ring	—	110·6 (2)

$-0{\cdot}21$ e $Å^{-3}$ (II). Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Atomic coordinates and equivalent isotropic temperature factors for (I) and (II) are given in Tables 1 and 2, respectively.* A comparison of bond distances and angles is presented in Table 3. Figs. 1 and 2 by *PLUTO* (Motherwell & Clegg, 1978) show the atom numbering for (I) and (II), respectively.

Related literature. The structure analyses are part of a study of the effects of *gem* electro captor and acceptor (*cd*) substitution on molecular deformation in dehydro dimers $(R_1R_2R_3C)_2$. The molecular geometry can be compared with that of other symmetric *cd*-tetrasubstituted or hexasubstituted ethanes (Parfonry, Tinant, Declercq & Van Meerssche, 1983) and with that of 1,1,2,2-ethanetetracarbonitrile (Declercq, Tinant, Parfonry & Van Meerssche, 1983).

* Lists of structure factors, H-atom parameters and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42870 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

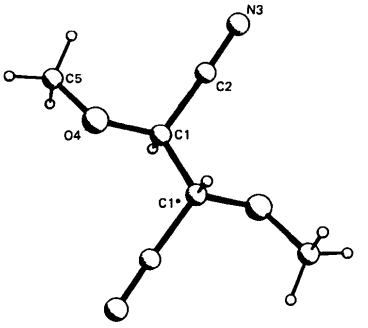

Fig. 1. View of the molecule (I) showing atom numbering.

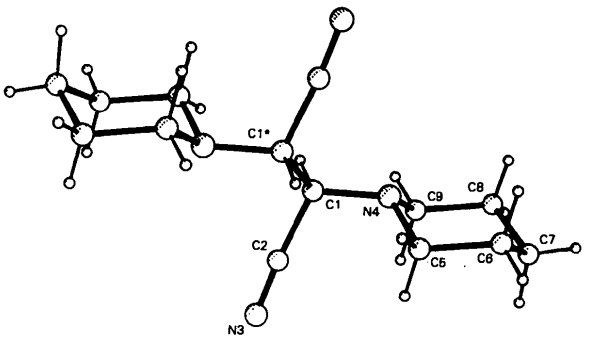

Fig. 2. View of the molecule (II) showing atom numbering.

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