shown in Table 2 in accordance with the atom-numbering scheme shown in Fig. 1 (I) and Fig. 2 (II).*

Related literature. The inclination angles between the least-squares planes of the carbamate and phenyl groups, 86·3 (I) and 82·5° (II), differ from related molecules including dimethyl 4,4′-methylenebis(phenylcarbamate) (Gardner & Blackwell, 1980) and bis(4-hydroxybutyl)-4,4′-methylenebis(phenyl carbamate) (Forcier & Blackwell, 1981). A structure reported by Born, Hocker, Paulus & Wolfel, (1981) shows a number of similarities.

We thank Dr Robert Saxon of American Cyanamide Company for providing the samples of *p*-TMXDI (Singh, Chang & Forgione, 1984). JPJ wishes to thank MTL and the US Army for an IPA fellowship and support of this work. JPJ also wishes to thank Dr E. M. Holt, Oklahoma State University, for her assistance and advice during the early stages of this work.

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The Structures of Dimethyl *N,N′*-*trans*-1,4-Cyclohexanedicarbamate (I) and Diethyl *N,N′*-*trans*-1,4-Cyclohexanedicarbamate (II)

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Abstract. (I) $C_{10}H_{18}N_2O_4$, $M_r = 230\cdot27$, monoclinic, $P2_1/c$, $a = 10\cdot563\ (2)$, $b = 7\cdot265\ (1)$, $c = 8\cdot375\ (1)$ Å, $\beta = 106\cdot87\ (1)°$, $V = 615\cdot0$ Å^3, $Z = 2$, $D_x = 1\cdot243$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0\cdot71073$ Å, $\mu = 0\cdot899$ cm^{-1}, $F(000) = 248$, room temperature. $R = 0\cdot058$, 1041 independent observed reflections. (II) $C_{12}H_{22}N_2O_4$, $M_r = 258\cdot32$, triclinic, $P\bar{1}$, $a = 8\cdot251\ (5)$, $b = 9\cdot284\ (5)$, $c = 12\cdot479\ (7)$ Å, $\alpha = 69\cdot30\ (1)$, $\beta = 108\cdot18\ (1)$, $\gamma = 68\cdot78\ (1)°$, $V = 719\cdot7$ Å^3, $Z = 2$, $D_x = 1\cdot192$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0\cdot71073$ Å, $\mu =$

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Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* (Å^2) *for* (I) *and* (II) *with e.s.d.'s in the least significant digit in parentheses*

	x	y	z	U_{eq}*
(I) $C_{10}H_{18}N_2O_4$				
O(1)	8653 (2)	620 (2)	2820 (2)	48·3 (4)
O(2)	7599 (2)	542 (2)	68 (2)	52·6 (4)
N(1)	7111 (2)	2673 (3)	1771 (2)	45·3 (4)
C(1)	7761 (2)	1231 (3)	1439 (2)	37·5 (4)
C(2)	6058 (2)	3615 (3)	519 (2)	39·6 (4)
C(3)	6380 (2)	5641 (4)	421 (3)	48·7 (5)
C(4)	4736 (2)	3386 (4)	885 (3)	49·3 (5)
C(5)	9436 (3)	−925 (4)	2614 (4)	67·9 (7)
(II) $C_{12}H_{22}N_2O_4$				
O(11)	1473 (4)	4246 (4)	2822 (3)	5·9 (1)
O(12)	1220 (5)	2687 (4)	1822 (4)	8·7 (1)
O(21)	3486 (4)	1146 (4)	6823 (3)	5·6 (1)
O(22)	3667 (5)	2977 (4)	7598 (3)	7·7 (1)
N(1)	−1522 (5)	4914 (4)	1491 (4)	5·3 (1)
N(2)	6464 (5)	529 (4)	8148 (4)	5·4 (1)
C(11)	−3001 (6)	4743 (5)	621 (4)	4·5 (2)
C(12)	−4804 (7)	6574 (6)	−517 (5)	5·4 (2)
C(13)	−3640 (8)	3661 (6)	1386 (5)	5·9 (2)
C(14)	422 (7)	3857 (6)	2003 (5)	5·2 (2)
C(15)	3674 (7)	2993 (7)	3559 (6)	8·5 (2)
C(16)	4571 (9)	3627 (9)	4300 (6)	10·8 (3)
C(21)	7926 (6)	697 (5)	9024 (5)	5·3 (2)
C(22)	9458 (7)	698 (6)	8629 (5)	5·4 (2)
C(23)	8939 (7)	−807 (6)	10443 (5)	5·9 (2)
C(24)	4489 (6)	1646 (6)	7541 (5)	5·1 (2)
C(25)	1353 (8)	2324 (7)	6033 (6)	8·0 (2)
C(26)	545 (8)	1622 (9)	5295 (6)	9·4 (3)

* $U_{eq} = \frac{1}{3}$ trace U_{ij}.

Table 2. *Selected bond lengths* (Å) *and bond angles* (°) *for* (I) *and* (II)

(I) $C_{10}H_{18}N_2O_4$		(II) $C_{12}H_{22}N_2O_4$	
C(2)—C(3)	1·518 (3)	C(11)—C(12)	1·504 (6)
C(2)—C(4)	1·523 (3)	C(11)—C(13)	1·490 (7)
C(1)—N(1)	1·326 (2)	C(15)—C(16)	1·422 (8)
C(1)—O(1)	1·338 (2)	C(21)—C(22)	1·493 (7)
C(1)—O(2)	1·218 (2)	C(21)—C(23)	1·506 (7)
C(2)—N(1)	1·459 (2)	C(25)—C(26)	1·439 (8)
C(5)—O(1)	1·434 (3)	C(11)—N(1)	1·458 (6)
		C(14)—N(1)	1·312 (6)
		C(21)—N(2)	1·452 (6)
		C(24)—N(2)	1·325 (6)
		C(14)—O(11)	1·365 (6)
		C(14)—O(12)	1·189 (5)
		C(15)—O(11)	1·472 (6)
		C(24)—O(21)	1·347 (6)
		C(24)—O(22)	1·215 (5)
		C(25)—O(21)	1·424 (6)
C(3)—C(2)—C(4)	110·5 (2)	C(12)—C(11)—C(13)	110·2 (4)
N(1)—C(2)—C(3)	111·0 (2)	C(22)—C(21)—C(23)	110·4 (4)
N(1)—C(2)—C(4)	110·9 (1)	N(1)—C(11)—C(12)	111·5 (5)
N(1)—C(1)—O(1)	111·0 (1)	N(1)—C(11)—C(13)	110·4 (5)
N(1)—C(1)—O(2)	125·6 (2)	N(2)—C(21)—C(22)	111·3 (5)
O(1)—C(1)—O(2)	123·4 (2)	N(2)—C(21)—C(23)	110·6 (5)
C(1)—N(1)—C(2)	123·6 (2)	O(11)—C(15)—C(16)	108·4 (5)
C(1)—O(1)—C(5)	116·2 (2)	O(21)—C(25)—C(26)	109·4 (5)
		O(11)—C(14)—N(1)	110·7 (5)
		O(12)—C(14)—N(1)	126·5 (6)
		O(21)—C(24)—N(2)	111·5 (5)
		O(22)—C(24)—N(2)	124·9 (6)
		O(11)—C(14)—O(12)	122·7 (5)
		O(21)—C(24)—O(22)	123·6 (5)
		C(11)—N(1)—C(14)	122·4 (4)
		C(21)—N(2)—C(24)	123·8 (5)
		C(14)—O(11)—C(15)	114·6 (4)
		C(24)—O(21)—C(25)	117·0 (4)

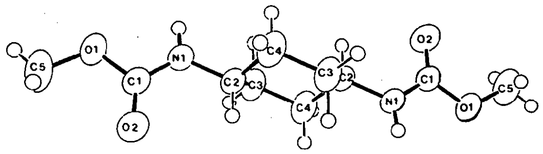

Fig. 1. Molecular drawing of $C_{10}H_{18}N_2O_4$.

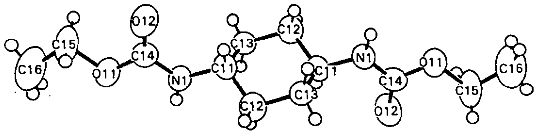

Fig. 2. Molecular drawing of $C_{12}H_{22}N_2O_4$.

0·835 cm^{-1}, $F(000) = 280$, room temperature. $R = 0·066$, 961 independent observed reflections. The angle between the least-sqares planes for the cyclohexane and carbamate groups is 87·5° in (I) and 82·3° in (II). In (I) a twofold axis relates the two halves of the molecule at $\frac{1}{2}$, $\frac{1}{2}$, 0 in the unit cell while (II) is centrosymmetric. The cyclohexane groups tend to stack in the *ab* plane nearly perpendicular to the *c* axis in (II) while in (I) the molecules are oriented in a cross-linked fashion.

Experimental. Clear colorless single crystals of dimensions 0·30 × 0·30 × 0·60 mm (I) and 0·30 × 0·40 × 0·60 mm (II), grown by slow evaporation of a mixture of 5 g of *trans*-1,4-cyclohexane diisocyanate (CHDI) (Zentner, 1987) after being refluxed in 100 ml of absolute methanol (I) or ethanol (II), was mounted on a 0·20 mm glass fiber in each case with the needle axis nearly parallel to the φ axis of a Nicolet *P*3*m* autodiffractometer. Cell dimensions and space-group data were determined by standard methods (Calabrese, 1980; Corfield, Doedens & Ibers, 1967). For each compound: cell constants from $\pm 2\theta$ values of 15 reflections in the range 15–30°; scan range between 2θ settings 0·8 (I) or 1·2° (II) above and below $K\alpha_1$ and $K\alpha_2$; 2θ range $4·0 \leq 2\theta \leq 60°$ (I), $4·0 \leq 2\theta \leq 50°$ (II); four standard reflections monitored every 500 (I) or 1000 (II) reflections; data points corrected for Lorentz–polarization effects. (I): 1803 independent reflections; index ranges $0 \leq h \leq 14$, $0 \leq k \leq 10$, $-11 \leq l \leq 11$. (II): 2673 independent reflections; index ranges $-9 \leq h \leq 9$, $-10 \leq k \leq 10$, $0 \leq l \leq 13$. Each structure was solved by direct methods using a modified version of *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), *SDP-Plus* (B. A. Frenz & Associates Inc., 1984) and *TEXRAY* 234 (Molecular Structure Corporation, 1984). O, N and C atoms anisotropic, hydrogen atoms from $\Delta\rho$ map refined isotropically for three cycles and subsequently held fixed; $\sum w(|F_o| - |F_c|)^2$ minimized; $w = 4F_o^2/(\sigma F_o^2)^2$, where $(\sigma F_o^2)^2 = [s^2(c + R^2B) + (pF_o^2)^2]/\mathrm{Lp}^2$ and p (ignorance factor used to downweight intense reflections) = 0·065 (I) or 0·050 (II) with $I > 3\sigma(I)$ (Corfield, Doedens & Ibers, 1967); no absorption corrections applied; features in final $\Delta\rho$ map $\pm 0{\cdot}20$ e Å^{-3}; scattering factors and anomalous-dispersion values were taken from standard sources (*International Tables for X-ray Crystallography*, 1974; Stewart, Davidson & Simpson, 1965). (I): R(109 variables) = 0·058 and wR = 0·087 for 1041 independent reflections; S = 0·06; $(\Delta/\sigma)_{\max}$ = 0·001. (II): R(163 variables) = 0·066 and wR = 0·068 for 961 independent reflections; S = 0·2; $(\Delta/\sigma)_{\max}$ = 0·001. Final atomic coordinates are listed in Table 1,* and bond lengths and angles in Table 2. Figs. 1 and 2 show perspective views of (I) and (II) with atomic numbering.

Related literature. The inclination angles between the least-squares planes of the cyclohexane and carbamate groups, 87·5 (I) and 82·3° (II), show similarities to structures reported by Jasinski, Desper, Zentner, Butcher & Day (1988). Other related molecules reported by Gardner & Blackwell (1980), Forcier & Blackwell (1981) and Born, Hocker, Paulus & Wolfel (1981) differ in this comparison but show a number of other similarities.

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Structure of Methyl 8,9-Epoxy-5,5-ethylenedioxy-7-oxo-11-methoxytricyclo[7.2.1.0^{4,10}]dodec-3-ene-8-carboxylate

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Abstract. $C_{17}H_{20}O_7$, M_r = 336·34, monoclinic, $C2/c$, a = 15·059 (6), b = 6·888 (2), c = 30·557 (12) Å, β = 94·30 (3)°, U = 3161 (2) Å^3, Z = 8, D_x = 1·413 g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ = 1·0 cm^{-1}, $F(000)$ = 1424, T = 295 K, R = 0·059 for 1169 reflections with $I \geq 1{\cdot}5\sigma(I)$. The carboxylate moiety is coplanar with the adjacent C—O bond of the epoxy group. The bond lengths and angles are as expected.

Experimental. X-ray data for a plate-shaped transparent colourless crystal (0·07 × 0·45 × 0·55 mm), glued on top of a glass fibre, were collected on an Enraf–Nonius CAD-4F diffractometer using Zr-filtered Mo $K\alpha$ radiation. The crystals were found to be poorly

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