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(*Z*)-α,β-Dimethoxystilbene

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Abstract. $C_{16}H_{16}O_2$, $M_r = 240.30$, orthorhombic, $P2_12_12_1$, $a = 7.569\,(1)$, $b = 9.308\,(1)$, $c = 18.502\,(2)$ Å, $V = 1303.5\,(3)$ Å^3, $Z = 4$, $D_x = 1.22$ g cm^{-3}, $\lambda(\text{Cu}\ K\alpha) = 1.5418$ Å, $\mu = 6.39$ cm^{-1}, $F(000) = 512$, $T = 291$ K, $R = 0.056$ for 2123 observed reflections. The central skeleton of the molecule exhibits a marked deviation from planarity. The dihedral angle between the two O—C(vinyl)—C(aromatic) planes is 11.6 (7)°. The phenyl rings are twisted out of the ethylenic bond plane by 34.2 (6) and 49.8 (6)°, respectively.

Experimental. Crystals were obtained by evaporation from chloroform. Parallelepiped crystal with dimensions 0.24 × 0.22 × 0.08 mm. Lattice parameters refined using 27 reflections in the range $5 \leq 2\theta \leq 50°$. Huber diffractometer and Rigaku RU200 rotating-anode generator, graphite-monochromatized Cu $K\alpha$ radiation. 2343 independent reflections with $\sin\theta/\lambda \leq 0.6$ Å^{-1}; $-8 \leq h \leq 9$, $0 \leq k \leq 11$, $0 \leq l \leq 22$, 2123 with $I \geq 2.5\sigma(I)$. Standard reflection $(10\overline{3})$ checked every 50 reflections; no significant deviation. Structure solved by direct methods using *SHELXS*86 (Sheldrick, 1985). H atoms in computed positions (C—H = 1.08 Å, H—C—H = 109.5°). Anisotropic least-squares refinement (*SHELX*76; Sheldrick, 1976) using *F*; H atoms isotropic with common refined temperature factor ($U = 0.090$ Å^2). $w = 1/(\sigma^2 + 0.04013F^2)$, $R = 0.056$, $wR = 0.063$, $S = 0.42$ for 2123 observed reflections. Final maximum shift to e.s.d. = 0.08. Maximum and minimum heights in final difference Fourier synthesis = 0.29 and −0.40 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV).

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

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	*y*	*z*	U_{eq}
C1	1986 (3)	9419 (2)	6447 (1)	45 (1)
C2	1948 (3)	9418 (2)	7165 (1)	46 (1)
O3	720 (2)	8622 (2)	6079 (1)	60 (1)
C4	−655 (4)	9461 (3)	5772 (2)	72 (1)
O5	451 (2)	8896 (2)	7503 (1)	63 (1)
C6	721 (4)	7766 (3)	8005 (2)	64 (1)
C7	3293 (3)	10145 (2)	5975 (1)	44 (1)
C8	4049 (3)	11467 (2)	6152 (1)	50 (1)
C9	5253 (4)	12126 (3)	5702 (2)	65 (1)
C10	5722 (4)	11462 (4)	5054 (2)	77 (1)
C11	4971 (5)	10184 (5)	4862 (1)	80 (1)
C12	3749 (4)	9509 (3)	5318 (1)	63 (1)
C13	3338 (3)	9988 (2)	7655 (1)	43 (1)
C14	2889 (3)	10910 (3)	8222 (1)	52 (1)
C15	4181 (4)	11414 (3)	8684 (1)	60 (1)
C16	5920 (4)	11029 (3)	8594 (1)	59 (1)
C17	6371 (3)	10114 (3)	8032 (1)	56 (1)
C18	5089 (3)	9590 (2)	7570 (1)	48 (1)

Table 2. *Bond distances* (Å) *and bond angles* (°)

C2—C1	1.328 (3)	C10—C9	1.396 (5)
O3—C1	1.390 (2)	C11—C10	1.365 (6)
C7—C1	1.483 (3)	C12—C11	1.400 (5)
O5—C2	1.382 (3)	C14—C13	1.398 (3)
C13—C2	1.487 (3)	C18—C13	1.385 (3)
C4—O3	1.420 (3)	C15—C14	1.381 (4)
C6—O5	1.418 (3)	C16—C15	1.374 (4)
C8—C7	1.396 (3)	C17—C16	1.387 (4)
C12—C7	1.396 (3)	C18—C17	1.382 (3)
C9—C8	1.377 (3)		
O3—C1—C2	118.3 (2)	C10—C9—C8	119.3 (3)
C7—C1—C2	127.1 (2)	C11—C10—C9	120.2 (3)
C7—C1—O3	114.5 (2)	C12—C11—C10	120.7 (3)
O5—C2—C1	118.0 (2)	C11—C12—C7	119.8 (3)
C13—C2—C1	126.5 (2)	C14—C13—C2	120.3 (2)
C13—C2—O5	115.4 (2)	C18—C13—C2	120.8 (2)
C4—O3—C1	114.1 (2)	C18—C13—C14	118.9 (2)
C6—O5—C2	116.1 (2)	C15—C14—C13	120.0 (2)
C8—C7—C1	122.5 (2)	C16—C15—C14	121.0 (2)
C12—C7—C1	119.0 (2)	C17—C16—C15	119.2 (2)
C12—C7—C8	118.5 (2)	C18—C17—C16	120.5 (2)
C9—C8—C7	121.5 (2)	C17—C18—C13	120.4 (2)

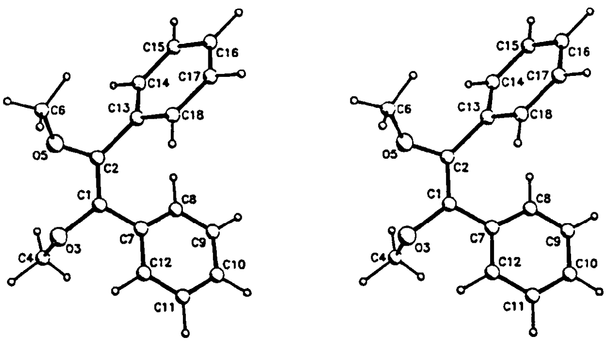

Fig. 1. Stereoscopic view of (Z)-α,β-dimethoxystilbene.

The atomic parameters are given in Table 1.* Bond lengths and bond angles are listed in Table 2. Fig. 1 is a stereoscopic view of the compound, showing the numbering of the atoms (*PLUTO*; Motherwell & Clegg, 1978).

Related literature. The compound has been synthetized following the procedure described by Merz & Tomahogh (1977). The structures of the sulfur analogues (E)- and (Z)-1,2-bis(methylthio)-1,2-diphenylethylene (Adiwidjaja, Kistenbrugger & Voss, 1981) and those of *cis*- and *trans*-1,2-bis(methoxyethoxy)-1,2-diphenylethylene (Soumillion, Weiler, De Man, Touillaux, Declercq & Tinant, 1989) have been reported. From dipole-moment measurements, Lumbroso, Lund & Simonet (1974) have discussed the *cis–trans* configurations and the conformation of the methoxy and phenyl groups in the title compound.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55362 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HA0102]

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Structure of Dimethyl Ceanothate

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Abstract. Methyl 2α-methoxycarbonyl-3β-hydroxy-A(1)-norlup-20(29)-en-28-oate, $C_{32}H_{50}O_5$, M_r = 514.7, orthorhombic, $P2_12_12_1$, $a = 9.795$ (2), b = 16.452 (2), c = 18.835 (2) Å, V = 3035.2 (2) Å^3, Z = 4, D_x = 1.13 g cm^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, μ = 5.52 cm^{-1}, $F(000)$ = 1128, T = 295 K, R = 0.049, wR = 0.057 for 2481 unique observed reflections [$I > 2\sigma(I)$]. Ring A is in a half-chair conformation and ring E is in an envelope conformation. Rings B, C and D have slightly distorted chair conformations with mean torsion angles of 54.8 (4), 58.4 (4) and 55.5 (4)°, respectively. The molecule is stabilized by van der Waals forces.

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