

angle of $15.0(3)^\circ$ with the double bond, quite similar to the value of 17.6° in (*E*)-1,2-bis(2-hydroxyphenyl)ethene. The C(9) phenyl ring forms a dihedral angle of $2.7(3)^\circ$ with the double bond, a value much closer to that of (*E*)-1,2-diphenylethene (3.3°) than to those of the 2-substituted phenyl derivatives.

Bond distances and angles are given in Table 2. Of note are the C(7)–C(8) double-bond distance of $1.320(4) \text{ \AA}$, and the angles at the two olefinic atoms. The chemically equivalent angles C(1)–C(7)–C(8), $128.1(3)^\circ$, and C(7)–C(8)–C(9), $127.0(3)^\circ$, are slightly larger than that found in (*E*)-1,2-bis(2-hydroxyphenyl)ethene, $125.2(3)^\circ$, but not significantly different from that found in (*E*)-1,2-diphenylethene, $126.7(2)^\circ$. The methoxy substituents are slightly non-coplanar with the phenyl rings, described by torsion angles C(1)–C(2)–O(1)–C(15), $173.1(5)^\circ$, and C(9)–C(10)–O(2)–C(16), $171.7(5)^\circ$. This contrasts with (*E*)-2,3-bis(2-methoxyphenyl)-2-butene, in which the corresponding torsion angle is $180.0(6)^\circ$, but compares well with (*Z*)-2,3-bis(2-methoxyphenyl)-2-butene, in which the two independent torsion angles are $176.8(9)$ and $171.5(9)^\circ$ (Fronczek *et al.*, 1984).

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(*Z*)-2,3-Diphenyl-2-butene,* $C_{16}H_{16}$

BY FRANK R. FRONCZEK, ANTHONY M. SWAN, JEFFREY A. CORKERN AND RICHARD D. GANDOUR†

Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803-1804, USA

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Abstract. $M_r = 208.3$, monoclinic, $P2_1/n$, $a = 10.217(3)$, $b = 8.703(1)$, $c = 14.342(4) \text{ \AA}$, $\beta = 95.67(2)^\circ$, $V = 1269.0(9) \text{ \AA}^3$, $Z = 4$, $D_x = 1.090 \text{ g cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $\mu(\text{Mo } K\alpha) = 0.57 \text{ cm}^{-1}$, $F(000) = 448$, $T = 296 \text{ K}$, $R = 0.050$ for 998 observations (of 1981 unique data). The molecule approximates symmetry 2, with the two phenyl rings forming dihedral angles of 59.1 and 49.7° with the best plane of the double bond. The double bond is twisted slightly away from planarity.

Introduction. In the course of our studies utilizing 2,3-bis(2-substituted-phenyl)-2-butenes as models for intramolecular reactions (Tirado-Rives, Oliver, Fronczek & Gandour, 1984; Fronczek, Oliver & Gandour,

1984), the crystal structure of the title compound has been determined. This crystal structure serves as a reference for comparison with more complex analogues and complements the recent report (Valle, Busetti & Galiazzo, 1981) of the crystal structure of the (*E*) isomer.

Experimental. Title compound prepared by a previously published procedure (Mukaiyama, Sato & Hanna, 1973), which produced a mixture of isomers. During removal under vacuum of traces of solvent from the mixture, the (*Z*) isomer sublimed. A suitable crystal was obtained from the sublimed material, m.p. 338 K [lit. m.p. 340 K (von Wessely & Welleba, 1941)]. Crystal $0.32 \times 0.52 \times 0.60 \text{ mm}$ mounted in a thin-walled glass capillary to prevent sublimation. Space group from systematic absences $0k0$ with k odd, $h0l$ with $h + l$ odd. Cell dimensions determined by least

* Alternative nomenclature: (*Z*)- α,β -dimethylstilbene.

† To whom correspondence should be addressed.

squares from setting angles of 25 reflections having $13^\circ > \theta > 11^\circ$. Enraf-Nonius CAD-4 diffractometer, Mo K α radiation, graphite monochromator. ω - 2θ scans designed to yield $I = 25\sigma(I)$. Scan rates varied, 0.56–5.0° min⁻¹. Data having $1^\circ < \theta < 24^\circ$, h 0–10, k 0–8, l -14–14 measured, corrected for background, Lorentz, and polarization effects, equivalent data averaged ($R_{\text{int}} = 0.022$). Crystal decay and absorption negligible. Structure solved using *MULTAN78* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), refined by full-matrix least squares based upon F using data with $I > 3\sigma(I)$, $w = [\sigma^2(|F|) + 0.04|F|^2]^{-1}$ and *Enraf-Nonius SDP* (Frenz & Okaya, 1980). Scattering factors of Cromer & Waber (1974). Non-H atoms anisotropic; H atoms located by ΔF map, fixed contributions with $B = 6.0 \text{ \AA}^2$. Final $R = 0.050$, $R_w = 0.068$ and $S = 1.84$ for 145 variables. Max. $\Delta/\sigma = 0.02$ in final cycle, largest residual density 0.17 e \AA^{-3} .

Discussion. The atomic parameters are given in Table 1.* Selected distances, angles, and torsion angles are given in Fig. 1.

The molecule has approximate symmetry 2. There is a distinct difference between the dihedral angles which the two phenyl rings make with the double bond. The molecule exhibits a very slight twist about the double bond. Distances and angles lie in the expected range of values. There are no unusually short intermolecular contacts less than 3.3 Å between heavy atoms.

A comparison can be made with (Z)-2,3-bis(2-methoxyphenyl)-2-butene (Fronczek, Oliver & Gandour, 1984). The distance between the two atoms of the double bond appears marginally longer for the title compound [compare 1.343 (4) with 1.310 (10) Å]. There are no significant differences among the bond angles. Noticeable differences occur in the dihedral angles which the phenyl rings form with the double bond (57.6 and 49.3° vs 71.6 and 68.2°); the title compound has the lower values. The twist in the double bond is less in the title compound [3.9 (5) compared with 9.8 (9)°]. The conclusion is that a methoxy substituent at the *ortho* position increases the dihedral angle and the twist angle because of buttressing of the methoxy group with the methyl group.

Comparisons cannot be made with the title compound and its (*E*) isomer since the latter crystal is disordered (Valle, Buseti & Galiazzo, 1981).

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* Lists of distances and angles, H-atom coordinates, anisotropic thermal parameters and structure factor amplitudes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39574 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Coordinates and equivalent isotropic thermal parameters*

$$B_{\text{eq}} = \frac{1}{3}(a^2B_{11} + b^2B_{22} + c^2B_{33} + abB_{12}\cos\gamma + acB_{13}\cos\beta + bcB_{23}\cos\alpha).$$

	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}}(\text{\AA}^2)$
C(1)	0.3117 (4)	0.6661 (4)	0.3436 (2)	5.49 (8)
C(2)	0.1870 (4)	0.6915 (5)	0.2996 (3)	6.39 (9)
C(3)	0.1173 (4)	0.8220 (5)	0.3202 (3)	6.7 (1)
C(4)	0.1743 (4)	0.9254 (5)	0.3848 (2)	6.33 (9)
C(5)	0.2986 (3)	0.9003 (4)	0.4296 (2)	5.12 (8)
C(6)	0.3691 (3)	0.7699 (4)	0.4094 (2)	4.45 (7)
C(7)	0.5025 (3)	0.7395 (4)	0.4584 (2)	4.83 (7)
C(8)	0.6098 (3)	0.7181 (4)	0.4130 (2)	5.30 (8)
C(9)	0.6068 (3)	0.7325 (4)	0.3086 (2)	4.98 (8)
C(10)	0.6634 (3)	0.6182 (5)	0.2570 (3)	6.16 (9)
C(11)	0.6601 (4)	0.6291 (5)	0.1603 (3)	7.0 (1)
C(12)	0.6016 (3)	0.7536 (5)	0.1133 (2)	6.41 (9)
C(13)	0.5473 (3)	0.8694 (5)	0.1637 (2)	6.10 (9)
C(14)	0.5512 (3)	0.8579 (4)	0.2605 (2)	5.45 (8)
C(15)	0.5046 (4)	0.7276 (5)	0.5635 (2)	6.29 (9)
C(16)	0.7424 (4)	0.6773 (5)	0.4636 (3)	7.2 (1)

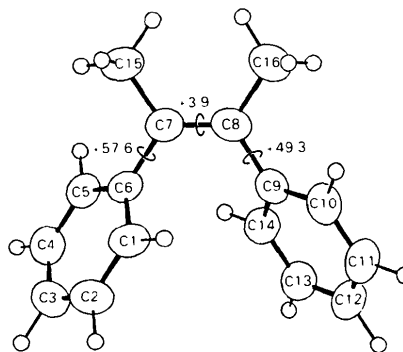


Fig. 1. Drawing of the title compound with selected torsion angles (e.s.d. 0.5°). Distances and angles, averaged over the two halves of the molecule, are C(7)–C(8) 1.343 (4), C(6)–C(7) 1.497 (3), C(7)–C(15) 1.512 (3) Å, C(6)–C(7)–C(8) 122.8 (4), C(6)–C(7)–C(15) 114.6 (7), C(8)–C(7)–C(15) 122.6 (3)°.

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