crystal packing arrangement in stereo form using *PLUTO* (Motherwell & Clegg, 1978).*

Related literature. The title compound belongs to the class of natural products known as lignans which contain the 2,3-dibenzylbutane skeleton. These compounds show strong antimitotic activity and many semi-synthetic derivatives of them have proven useful as anticancer drugs (Gupta & Ross, 1989). The synthesis of this compound serves as an initial step in the attempted design of more specific and potent compounds. Recently the crystal structure of a thymidine derivative of DMEP exhibiting POD-like antimitotic activity was reported by Sicheri, Derry, Gupta & Yang (1991).

Structure–activity studies of podophyllotoxin and its derivatives, including 4′-demethylepipodophyllotoxin, on *in vitro* microtubule assembly have been investigated by Lokie, Brewer, Sternlicht, Gensler & Horwitz (1978).

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Structure of 2-Methoxy-4-nitroaniline

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Abstract. $C_7H_8N_2O_3$, $M_r = 168.2$, monoclinic, $P2_1/a$, $a = 7.086\,(1)$, $b = 15.030\,(2)$, $c = 7.214\,(1)$ Å, $\beta = 91.75\,(1)°$, $V = 768.08\,(2)$ Å^3, $Z = 4$, $D_m = 1.42$ (by flotation), $D_x = 1.454$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 1.082$ cm^{-1}, $F(000) = 352$, $T = 295$ K, $R = 0.0362$, $wR = 0.0390$ for 675 reflections. The structure consists of planar molecules with intermolecular hydrogen bonding. The molecular geometry suggests the contribution of a quinonoid resonance form to the structure due to conjugation effects, as found in other *p*-nitroaniline derivatives [Ploug-Sørenson & Krogh Andersen (1982). *Acta Cryst.* **B38**, 671–673].

Experimental. A crystal of the title compound measuring 0.15 × 0.10 × 0.5 mm was used for intensity data collection on a Siemens *R*3*m* diffractometer with graphite-monochromated Mo $K\alpha$ radiation, $\omega/2\theta$-scan mode, scan speed 1° min^{-1}, $\theta \le 23.5°$. Cell constants obtained from the least-squares fit of 2θ values for 22 reflections ($12 \le 2\theta \le 35°$). Intensities were corrected for Lorentz and polarization effects, no correction for absorption. Total reflections 1115, unique 1039 ($R_{\text{int}} = 0.0209$) and index range of $h = -10$ to 10, $k = 0$ to 22, $l = 0$ to 10 ($2\theta < 48°$). Three standard reflections ($\bar{1}71$, 022, 152) measured periodically displayed intensity variation < 3%. Structure solved using the *SHELXTL* program (Sheldrick, 1983); 675 reflections at 4σ level were used for refinement. $w(|F_o| - |F_c|)^2$ minimized where $w = 1.000[\sigma^2(F) + 0.002352(F^2)]$. Final stage of refinement performed with 111 variables including

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

$U_{eq} = \frac{1}{3} \times$ trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
C4	0.7847 (4)	0.1502 (2)	1.0697 (4)	460 (13)
C3	0.7189 (4)	0.1159 (2)	0.8983 (4)	468 (13)
C2	0.6627 (4)	0.1715 (2)	0.7577 (4)	488 (13)
C1	0.6715 (4)	0.2628 (2)	0.7861 (4)	399 (24)
C6	0.7332 (4)	0.2984 (2)	0.9532 (4)	475 (14)
C5	0.7888 (4)	0.2421 (2)	1.0943 (4)	491 (13)
N2	0.8433 (4)	0.0945 (2)	1.2067 (3)	664 (14)
O3	0.7195 (3)	0.0253 (1)	0.8899 (3)	666 (11)
C7	0.6523 (6)	−0.0133 (2)	0.7214 (5)	870 (21)
N1	0.6133 (4)	0.3203 (2)	0.6373 (4)	566 (12)
O1	0.5500 (4)	0.2876 (2)	0.4921 (3)	771 (11)
O2	0.6249 (4)	0.4016 (2)	0.6583 (3)	791 (12)

Table 2. *Bond lengths* (Å), *bond angles* (°) *and intermolecular hydrogen bonding* (Å, °) *with e.s.d.'s in parentheses*

C4—C3	1.406 (4)	C5—C4—N2	121.1 (3)
C4—C5	1.393 (4)	C3—C4—N2	120.2 (3)
C4—N2	1.351 (4)	C3—C4—C5	118.7 (3)
C3—C2	1.364 (4)	C4—C3—O3	113.8 (2)
C3—O3	1.363 (3)	C4—C3—C2	120.7 (3)
C2—C1	1.389 (4)	C2—C3—O3	125.5 (3)
C1—C6	1.378 (4)	C3—C2—C1	119.0 (3)
C1—N1	1.429 (4)	C2—C1—N1	118.4 (3)
C6—C5	1.373 (4)	C2—C1—C6	121.6 (3)
O3—C7	1.416 (4)	C6—C1—N1	119.9 (3)
N1—O1	1.221 (3)	C1—C6—C5	119.1 (3)
N1—O2	1.234 (4)	C4—C5—C6	121.8 (3)

N(2)—O(1^{i})	3.056 (4)	N(2)—H(2*B*)···O(1)	153
H(2*B*)—O(1^{i})	2.228 (4)		
N(2)—O(2^{ii})	3.065 (4)	N(2)—H(2*A*)···O(2)	142
H(2*A*)—O(2^{ii})	2.303 (4)		

Symmetry code: (i) = $\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$; (ii) = $\frac{3}{2} - x, y - \frac{1}{2}, 2 - z$.

all positional parameters, anisotropic thermal parameters for the non-H atoms, isotropic for H atoms and one scale factor. H atoms in calculated positions. Large *U* values for the methyl group may indicate certain disorder; convergence yielded $R = 0.0362$, $wR = 0.0390$, and $R = 0.0622$, $wR = 0630$ for all 1039 data, $(\Delta/\sigma)_{max} = 0.081$. Maximum and minimum in final $\Delta\rho$ map = 0.13 and -0.17 e $Å^{-3}$, $S = 0.596$. Positional and isotropic thermal parameters are listed in Table 1,* bond lengths and angles are in Table 2. Fig. 1 illustrates the molecular structure with atomic labelling, Fig. 2 displays molecular packing. Refinements performed with *SHELXTL* (Sheldrick, 1983). Interatomic distances and angles, torsion angles and hydrogen-bond parameters computed using *PARST* (Nardelli, 1983). All computations performed on a VAX Workstation 3100 of our laboratory. Atomic scattering factors were those of *SHELX*. Drawings computed using the program *MOLDRAW* (Ugliengo, Borzani & Viterbo, 1988).

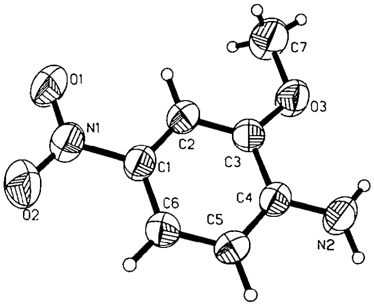

Fig. 1. Molecular structure with atomic labelling.

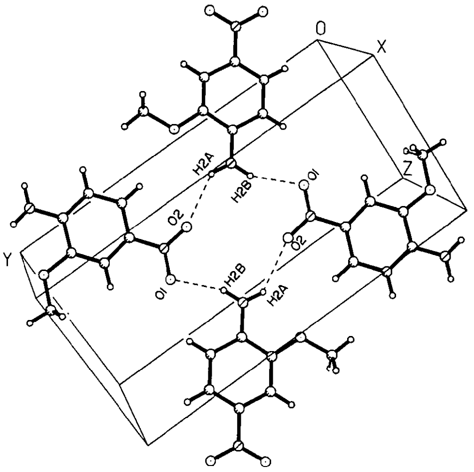

Fig. 2. Packing of the molecules.

Related literature. Structures of *p*-nitroaniline (Trueblood, Goldish & Donohue, 1961; Colapietro, Domenicano, Marciante & Portalone, 1982), *N*,*N*-dimethyl-*p*-nitroaniline (Mak & Trotter, 1965), *N*-(*p*-nitrophenyl)ethylenediamine (Kaida, Wakita, Shimizu, Sonoda, Miki & Kasai, 1989) and 2,4-dinitroaniline (Prasad, Gabe & Le Page, 1982) have similarities.

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Structure of 4′-Methoxychalcone

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Abstract. 1-(4-Methoxyphenyl)-3-phenyl-2-propen-1-one, $C_{16}H_{14}O_2$, $M_r = 238.29$, orthorhombic, $Pbca$, $a = 10.891\,(2)$, $b = 30.507\,(2)$, $c = 7.499\,(3)$ Å, $V = 2491.6$ Å^3, $Z = 8$, $D_x = 1.27$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 0.8$ cm^{-1}, $F(000) = 1008$, room temperature, final $R = 0.053$ for 1242 observed reflections with $I > 3\sigma(I)$. The torsion angle O(2)—C(2)—C(3)—C(4) of the C_2H_2CO group is $-17.7\,(2)$°. The dihedral angle between the phenyl rings is 33.3°.

Experimental. The title compound was prepared by the acyloin condensation method from benzaldehyde and 4-methoxyacetophenone at room temperature (Migridichian, 1957). The ^{1}H NMR spectra were recorded on a Varian FT-80*A* NMR spectrometer operating at 80 MHz with internal deuterium lock. The spectra were measured in $CDCl_3$ at 298 K. δ: 3.89 (3H, *s*, —OCH_3); 7.00–7.70 (7H, *m*, $C_6H_5C_2H_2$—); 6.87, 6.97, 7.91, 8.01 (4H, *q*, —O—C_6H_4—). The crystals for X-ray work were obtained from ethanol solution. A colorless transparent block crystal with approximate dimensions 1.5 × 0.5 × 0.3 mm was mounted on a glass fiber in a random orientation. Preliminary examination and intensity data collection were performed on a Rigaku MSC/AFC-5*R* diffractometer with graphite-monochromated Mo $K\alpha$ radiation. Lattice parameters were determined by least squares from 20 reflections with $18 < 2\theta < 22$°. A total of 2507 unique reflections were collected in the range $1 < \theta < 25$° ($0 < h < 12$, $0 < k < 32$, $0 < l < 8$) by the ω–2θ scan technique, ω-scan width $(1.008 + 0.35\tan\theta)$°, scan speed 16° min^{-1}. 1242 reflections with $I > 3\sigma(I)$ were used for structure determination. Three standard reflections were monitored every 150 measurements. The correction factors based on variations in the monitor reflections ranged from 0.986 to 1.051.

The data were corrected for Lorentz and polarization factors. An empirical absorption correction based on a series of ψ scans and the program *DIFABS* (Walker & Stuart, 1983) was applied. Relative transmission coefficients ranged from 0.830 to 1.357 with an average value of 0.995. The structure was solved by direct methods. Atomic scattering factors and f', f'' values were taken from Cromer & Waber (1974). The H atoms were located from difference Fourier maps. The scale factor and positional and anisotropic thermal parameters for non-H atoms were refined by full-matrix least-squares methods, with 163 parameters being refined in the final cycle. The function minimized was $\sum w(|F_o| - |F_c|)^2$, using weights $w = 1/\sigma^2(F_o)$. The final discrepancy factors were $R = 0.53$, $wR = 0.53$, $S = 1.37$, $(\Delta/\sigma)_{\max} = 0.01$. The maximum $\Delta\rho$ was 0.17 e Å^{-3} with an estimated error based on ΔF of 0.04 e Å^{-3}. All calculations were performed on a VAX computer using *SDP*/*VAX* (Frenz, 1978).

The final atomic coordinates and thermal parameters are given in Table 1. Bond lengths and angles are listed in Table 2 and several least-squares planes are given in Table 3. The molecular configuration and the packing of molecules in the unit cell are shown in Figs. 1 and 2, respectively.† The torsional angle is $-17.7\,(2)$° for O(2)—C(2)—C(3)—C(4) of the C_2H_2CO group. The H atoms are *trans* in the —C═C— group and the dihedral angle between

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† Lists of structure factors, anisotropic thermal parameters, distances and angles involving H atoms, intermolecular bond distances, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54696 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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