been reported (Poleti, Stojaković, Prelesnik & Manojlović-Muir, 1990).

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Structure of 2-(4-Dimethylaminobenzylidene)cyclohexanone

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(*Received* 12 *February* 1990; *accepted* 2 *May* 1990)

Abstract. $C_{15}H_{19}NO$, $M_r = 229{\cdot}32$, monoclinic, $P2_1/c$, $a = 7{\cdot}179\ (4)$, $b = 11{\cdot}002\ (2)$, $c = 16{\cdot}110\ (3)$ Å, $\beta = 95{\cdot}15\ (4)°$, $V = 1267{\cdot}25$ Å^3, $Z = 4$, $D_x = 1{\cdot}201$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0{\cdot}59$ mm^{-1}, $F(000) = 496$, $T = 287$ K, $R = 0{\cdot}044$ ($wR = 0{\cdot}045$) for 1921 observed reflections. The cyclohexanone ring exhibits a chair conformation, flattened at the ketone end. The nonbonded steric strain between H atoms on the cyclohexanone and phenyl rings causes increases in the bond angles at the C atoms joining the rings, and rotation of the phenyl group about the C—Ph bond, at the expense of the conjugation energy of the system. The dimethylamino substituent, being an electron-donating group, makes the internal aromatic angle smaller than 120°.

Experimental. The synthesis of the title compound has been reported previously (Smith, Dimmock & Turner, 1973), m.p. 400–401 K. Orange-plate crystal, recrystallized from ethanol, dimensions 0·05 × 0·25 × 0·33 mm. The cell parameters were obtained by least squares using 25 reflections with $14{\cdot}93 < \theta < 22{\cdot}03°$. Enraf–Nonius CAD-4 diffractometer used for data collection, 2601 unique reflections, $-8 \le h \le 8$, $0 \le k \le 13$, $0 \le l \le 20$, $[(\sin\theta)/\lambda]_{max} = 0{\cdot}62653$ Å^{-1}. Three monitoring reflections, intensity constant to within 1·4%. No absorption correction. Merging R based on intensities of 0·0050 for 223 replicate reflections. Structure solved by direct methods using *XTAL2*·6 (Hall & Stewart, 1989), all non-H atoms found on E map and refined anisotropically; H atoms found on ΔF map and refined isotropically. 1921 reflections with $I > 2\sigma(I)$ used in refinement. $R = 0{\cdot}044$, $wR = 0{\cdot}045$ [$w = 1/\sigma^2(F)$], $S = 2{\cdot}34$ for 1921 observed reflections. 231 parameters refined and F magnitudes used in the refinement. Extinction correction included and secondary-extinction coefficient $g = 2{\cdot}8\ (6) \times 10^{-5}$. Final $(\Delta/\sigma)_{av} = 0{\cdot}026$, $(\Delta/\sigma)_{max} = 0{\cdot}36$. Maximum and minimum $\Delta\rho$ in final difference map of +0·18 and −0·15 e Å^{-3}, respectively. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). All calculations performed on a VAX6330 computer at the University of Saskatchewan.

The atomic parameters are summarized in Table 1.† Bond distances and angles are listed in Table 2. Fig. 1 is an *ORTEP* drawing (Johnson, 1976) of the title compound and Fig. 2 shows the packing in the unit cell.

Related literature. Other structures in this series of cyclic conjugated benzylidene ketones, which have various cytotoxicities towards P388 leukemia cells (Dimmock, Arora, Wonko, Hamon, Quail, Jia, Warrington, Fang & Lee, 1989; Dimmock, Arora, Jia,

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0108-2701/90/122467-02$03.00

† Lists of structure amplitudes, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53057 (18 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional coordinates and equivalent isotropic thermal parameters with e.s.d.'s in parentheses*

$U_{eq} = (U_{11} + U_{22}\sin^2\beta + U_{33} + 2U_{13}\cos\beta)/3\sin^2\beta$.

	x	y	z	U_{eq}(Å^2)
O	0·6356 (2)	−0·2013 (1)	0·09599 (9)	0·0749 (9)
N	−0·1933 (2)	0·0103 (2)	0·3968 (1)	0·072 (1)
C1	0·6488 (3)	−0·0916 (2)	0·1058 (1)	0·0543 (9)
C2	0·7938 (3)	−0·0230 (2)	0·0626 (1)	0·068 (1)
C3	0·8415 (3)	0·1032 (2)	0·0971 (2)	0·068 (1)
C4	0·6632 (3)	0·1718 (2)	0·1074 (1)	0·060 (1)
C5	0·5555 (3)	0·1102 (2)	0·1730 (1)	0·056 (1)
C6	0·5220 (2)	−0·0233 (1)	0·1578 (1)	0·0490 (9)
C7	0·3822 (2)	−0·0879 (2)	0·1867 (1)	0·0504 (9)
C8	0·2381 (2)	−0·0549 (1)	0·2404 (1)	0·0472 (8)
C9	0·2410 (2)	0·0459 (2)	0·2934 (1)	0·0494 (9)
C10	0·1009 (2)	0·0669 (2)	0·3451 (1)	0·0510 (9)
C11	−0·0529 (2)	−0·0113 (2)	0·3461 (1)	0·0510 (9)
C12	−0·0564 (2)	−0·1127 (2)	0·2937 (1)	0·058 (1)
C13	0·0853 (3)	−0·1336 (2)	0·2438 (1)	0·055 (1)
C14	−0·1920 (4)	0·1148 (2)	0·4501 (2)	0·074 (1)
C15	−0·3326 (4)	−0·0824 (3)	0·4084 (2)	0·089 (2)

Table 2. *Bond distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

O—C1	1·220 (2)	C5—C6	1·504 (2)
N—C11	1·374 (2)	C6—C7	1·347 (2)
N—C14	1·435 (3)	C7—C8	1·453 (2)
N—C15	1·452 (4)	C8—C9	1·398 (2)
C1—C2	1·505 (3)	C8—C13	1·402 (2)
C1—C6	1·494 (2)	C9—C10	1·382 (3)
C2—C3	1·522 (3)	C10—C11	1·401 (2)
C3—C4	1·508 (3)	C11—C12	1·398 (3)
C4—C5	1·523 (3)	C12—C13	1·372 (3)
C11—N—C14	121·9 (2)	C5—C6—C7	124·9 (2)
C11—N—C15	120·3 (2)	C6—C7—C8	131·8 (2)
C14—N—C15	117·0 (2)	C7—C8—C9	126·1 (2)
O—C1—C2	119·0 (2)	C7—C8—C13	118·0 (2)
O—C1—C6	121·7 (2)	C9—C8—C13	115·8 (2)
C2—C1—C6	119·2 (2)	C8—C9—C10	121·9 (2)
C1—C2—C3	115·5 (2)	C9—C10—C11	121·4 (2)
C2—C3—C4	109·3 (2)	N—C11—C10	121·4 (2)
C3—C4—C5	110·0 (2)	N—C11—C12	121·5 (2)
C4—C5—C6	113·9 (2)	C10—C11—C12	117·0 (2)
C1—C6—C5	119·1 (2)	C11—C12—C13	120·9 (2)
C1—C6—C7	116·0 (1)	C8—C13—C12	122·9 (2)

Quail, Warrington & Fang, 1989) have been reported previously (Jia, Quail, Arora & Dimmock, 1988, 1989*a*,*b*,*c*,*d*). The title compound shows similar geometrical features to those of related molecules, mainly as a result of steric strains (Tokuno, Matsui, Miyoshi, Asao, Ohashi & Kihara, 1986). The aromatic angle C10—C11—C12 is substantially smaller than 120° due to the strong electron-donating effect of the dimethylamino group (Carter, McPhail & Sim, 1966; Hope, 1969; Jia, Quail, Arora & Dimmock, 1989*a*).

ZJ thanks the University of Saskatchewan for financial support through a graduate scholarship. The assistance of Mr G. Tulloch in the preliminary stage of this work is gratefully acknowledged. We thank Dr L. T. J. Delbaere for the use of facilities for collecting data.

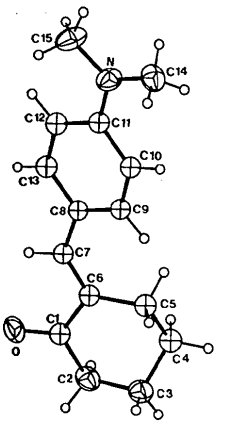

Fig. 1. *ORTEP* (Johnson, 1976) view of title compound with atomic numbering.

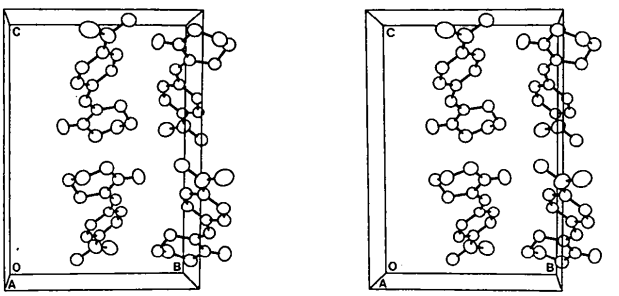

Fig. 2. Stereoscopic view showing the packing in the unit cell. H atoms are omitted for clarity.

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