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7,8-Benzochroman-4-one*

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(*Received* 30 *September* 1985; *accepted* 11 *February* 1986)

Abstract. $C_{13}H_{10}O_2$, $M_r = 198\cdot2$, monoclinic, $C2/c$, $a = 37\cdot915$ (4), $b = 6\cdot2466$ (3), $c = 8\cdot367$ (1) Å, $\beta = 100\cdot418$ (5)°, $V = 1949\cdot0$ (3) Å^3, $Z = 8$, $D_m = 1\cdot33$ (2) (flotation), $D_x = 1\cdot350$ Mg m^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1\cdot5418$ Å, $\mu = 0\cdot64$ mm^{-1}, $F(000) = 832$, $T = 294$ K, $R = 0\cdot062$ for 1289 observed reflections. The molecular geometry is similar to that observed in comparable systems. The dihydropyran ring system is a modified half-chair distorted toward the *d,e*-diplanar arrangement. The two benzene rings in the naphthalene group are planar. The crystal packing is mainly stabilized by van der Waals interactions.

Introduction. Chromanones are potential synthons for the construction of many important oxygen heterocycles. The crystal structure of the title compound has been determined as an aid to understanding the conformation of the dihydropyran ring in heterocycles.

Experimental. Crystals from benzene–hexane mixture, CAD-4 diffractometer, crystal dimensions $0\cdot15 \times 0\cdot13 \times 0\cdot14$ mm, monochromatized Cu $K\alpha$ radiation, cell parameters from $\sin^2\theta$ values for 25 reflections (θ range 40–50°), intensity data for $0 < \theta < 75°$, ω–$2(2/6)\theta$ scans, ω-scan angle $(1\cdot10 + 0\cdot24\tan\theta)°$, extended by 25% in each direction for background, scan speeds 1 to 10° min^{-1}, horizontal aperture $(2\cdot0 + \tan\theta)$ mm, vertical aperture 4 mm, three standard reflections, <1% intensity variation, Lp but no absorption correction; 2234 reflections (h 0→47, k 0→7, l −10→10, 1289 (58%) with $I \geq 3\sigma(I)$, $\sigma^2(I) = C + 2B + [0\cdot04\ (C-B)]^2$, C = scan count, B = time-corrected background. Direct methods with *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). An E map calculated from the set of phases with the highest figure of merit revealed the structure. Full-matrix least squares on F. Anisotropic temperature factors for C and O atoms, isotropic for H. H positions from difference map. $w = [\sigma^2(F_o) + 0\cdot0027\,F_o^2]^{-1}$, final $R = 0\cdot062$, $wR = 0\cdot072$ for 1289 observed reflections; $R = 0\cdot081$ for all 2234 reflections; $S = 1\cdot82$. $(\Delta/\sigma)_{\max} = 0\cdot52$, final ΔF map featureless, $\Delta\rho$ excursions $-0\cdot27$, $0\cdot29$ e Å^{-3}. No correction for secondary extinction, scattering factors as in *SHELX*76 (Sheldrick, 1976). Calculations performed on an IBM 370 computer.

Discussion. Final atomic parameters are in Table 1.§ Bond distances and angles are given in Fig. 1. A perspective view of the molecule is shown in Fig. 2. The values of bond lengths and angles are similar to those observed in other comparable systems.

The ether oxygen O(1) shows a tendency to be coplanar with the benzene ring [C(7)—C(12)—C(13)—O(1), 178·5 (4); C(5)—C(4)—C(13)—O(1), −179·8 (4)°] causing an enlargement of the angle O(1)—C(13)—C(4), 123·5 (3)°, and a narrowing of the

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* IUPAC name: 2,3-dihydro-4*H*-naphtho[2,1-*b*]pyran-4-one.

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‡ Contribution No. 679.

§ Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42826 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0108-2701/86/081043-02$01.50

Table 1. *Fractional positional parameters and equivalent isotropic thermal parameters*

$$B_{eq} = \tfrac{8}{3}\pi^2(U_{11} + U_{22} + U_{33}).$$

	x	y	z	B_{eq}(Å^2)
O(1)	0·1606 (1)	0·5052 (6)	0·6190 (4)	4·3 (3)
O(2)	0·2110 (1)	0·0365 (7)	0·9162 (6)	5·9 (6)
C(1)	0·1944 (2)	0·5459 (8)	0·7283 (9)	5·7 (9)
C(2)	0·2167 (1)	0·3478 (8)	0·7570 (9)	5·6 (9)
C(3)	0·1964 (1)	0·1738 (8)	0·8246 (7)	4·4 (7)
C(4)	0·1574 (1)	0·1745 (7)	0·7627 (6)	3·7 (4)
C(5)	0·1357 (1)	0·0028 (8)	0·7988 (6)	4·4 (7)
C(6)	0·1006 (1)	−0·0075 (9)	0·7338 (7)	4·4 (7)
C(7)	0·0838 (2)	0·1552 (9)	0·6275 (6)	3·5 (7)
C(8)	0·0475 (1)	0·1505 (9)	0·5573 (7)	4·7 (6)
C(9)	0·0322 (1)	0·3096 (9)	0·4570 (7)	5·1 (7)
C(10)	0·0526 (1)	0·4842 (9)	0·4222 (7)	4·9 (8)
C(11)	0·0883 (1)	0·4961 (8)	0·4876 (6)	4·1 (4)
C(12)	0·1048 (1)	0·3323 (7)	0·5919 (5)	3·5 (4)
C(13)	0·1421 (1)	0·3364 (7)	0·6603 (5)	3·5 (3)

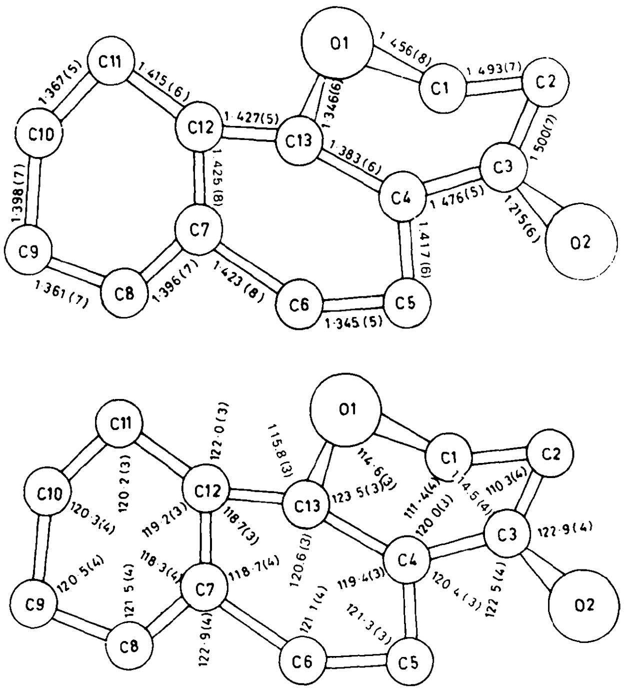

Fig. 1. Numbering scheme, bond distances (Å) and angles (°).

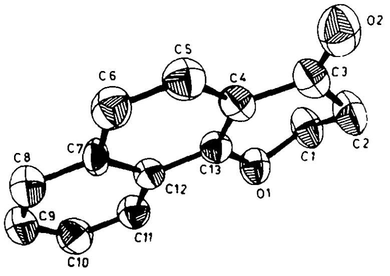

Fig. 2. *ORTEP* drawing (Johnson, 1976) of the title compound. Thermal ellipsoids are at the 50% probability level.

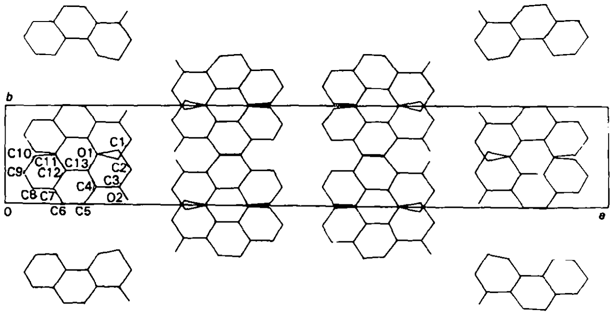

Fig. 3. Molecular packing of the title compound viewed along the *c* axis.

angle O(1)—C(13)—C(12), 115·8 (3)°. This tendency could be justified by some degree of conjugation between the oxygen [O(1)] and the benzene ring, giving rise to some shortening of C(ar)—O(1) [1·346 (6) Å]. This bond shortening has been found to be a common feature in the solid-state structures of a variety of compounds incorporating the pyran ring (Valente & Hodgson, 1979; Valente & Schomaker, 1984; Ponnuswamy & Trotter, 1984) and the anisole moiety (Domiano, Nardelli, Balsamo, Macchia & Macchia, 1979).

The conformation of the dihydropyran is a modified half-chair distorted toward the *d,e*-diplanar arrangement [C(2)—C(3)—C(4)—C(13) −4·5 (6); C(3)—C(4)—C(13)—O(1) −3·9 (6)°]. The two benzene rings in the naphthalene group are planar [$\sum(\Delta/\sigma)^2 = 0{\cdot}5$ and 13·4].

The molecular packing projected along the *ab* plane is shown in Fig. 3. The molecules are held in the crystal mainly by van der Waals interactions.

One of us (KR) thanks CSIR (India) for the award of a Senior Research Fellowship.

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