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2*H*-Chromen-4(3*H*)-one

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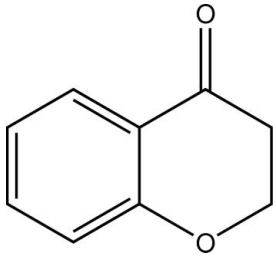
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.001 Å; R factor = 0.037; wR factor = 0.107; data-to-parameter ratio = 17.7.

In the title compound, $C_9H_8O_2$, a benzo-annulated heterocyclic ketone, the non-aromatic six-membered ring adopts an E_2 conformation. In the crystal, C—H···O contacts connect the molecules into double sheets perpendicular to the crystallographic a axis. The centroid–centroid distance for two π-systems is 3.7699 (6) Å.

Related literature

For the structure of a chromium(0) compound containing the title compound as a ligand, see: Stewart *et al.* (1984). For graph-set analysis of hydrogen bonds, see: Etter *et al.* (1990); Bernstein *et al.* (1995). For puckering analysis, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_9H_8O_2$ M_r = 148.15
Monoclinic, $P2_1/c$
a = 7.5538 (4) Å
b = 8.0896 (4) Å
c = 13.0410 (6) Å
β = 115.364 (3)°
V = 720.08 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 200 K
0.48 × 0.41 × 0.29 mm

Data collection

Bruker APEXII CCD diffractometer
6367 measured reflections
1774 independent reflections
1578 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.107
S = 1.05
1774 reflections
100 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H11···O2^{i}	0.99	2.53	3.4674 (13)	157
C1—H12···O2^{ii}	0.99	2.56	3.3934 (15)	141

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

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2010); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae,*et al.*, 2006); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

The authors thank Mr Raynard Fourie for helpful discussions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2060).

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supporting information

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S1. Comment

In general, saturated, six-membered carbocycles and heterocycles adopt energetically favourable chair- or boat-conformations in solution and in the solid state although a variety of other conformations such as half-chair- or twist-forms are available. The annulation of aromatic rings can influence the conformation of such ring-systems and "freeze" one of the less common conformations. In our continued interest in effects of substituents and annulation of differently-substituted aromatic systems on the conformation of six-, seven- and eight-membered ring systems, we determined the crystal structure of the title compound to enable comparative studies. As of today, only one structural analysis of a chromium(0)-compound featuring the title compound as a ligand is apparent in the literature (Stewart *et al.* 1984).

The heterocyclic six-membered ring adopts an E_2 conformation with carbon atom C1 acting as the *envelope*-atom. The latter one is displaced by 0.337 (1) Å from the least-squares plane defined by the atoms of the heterocycle. The least-squares planes defined by the carbon atoms of the phenyl ring as well as the skeletal atoms of the heterocycle intersect at an angle of 7.73 (6)°.

In the crystal structure, C–H···O contacts whose ranges fall by about 0.2 Å below the sum of van-der-Waals radii of the atoms participating are observed. These include both H atoms of the methylene group in *ortho*-position to the intracyclic O atom as donor atoms and exclusively the O atom of the carbonyl group as acceptor (Fig. 2). In total, the molecules are connected to double layers perpendicular to the crystallographic *a* axis. In terms of graph-set analysis (Etter *et al.*, 1990; Bernstein *et al.*, 1995) the descriptor for these contacts on the unitary level is *C*(5)*C*(5). The shortest $C_g\cdots C_g$-distance for two π-systems was measured at 3.7699 (6) Å.

The packing of the title compound is shown in Figure 3.

S2. Experimental

The compound was obtained commercially (Aldrich). Crystals suitable for the X-ray diffraction study were taken directly from the provided product.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å for aromatic C atoms and C—H 0.99 Å for aliphatic C atoms) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C).

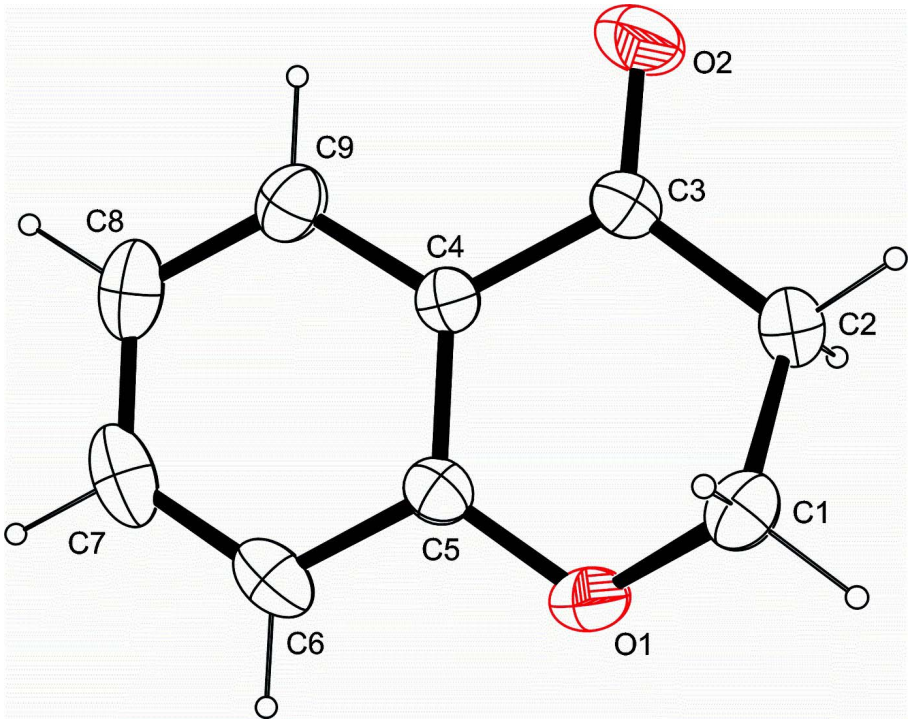

Figure 1

The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level).

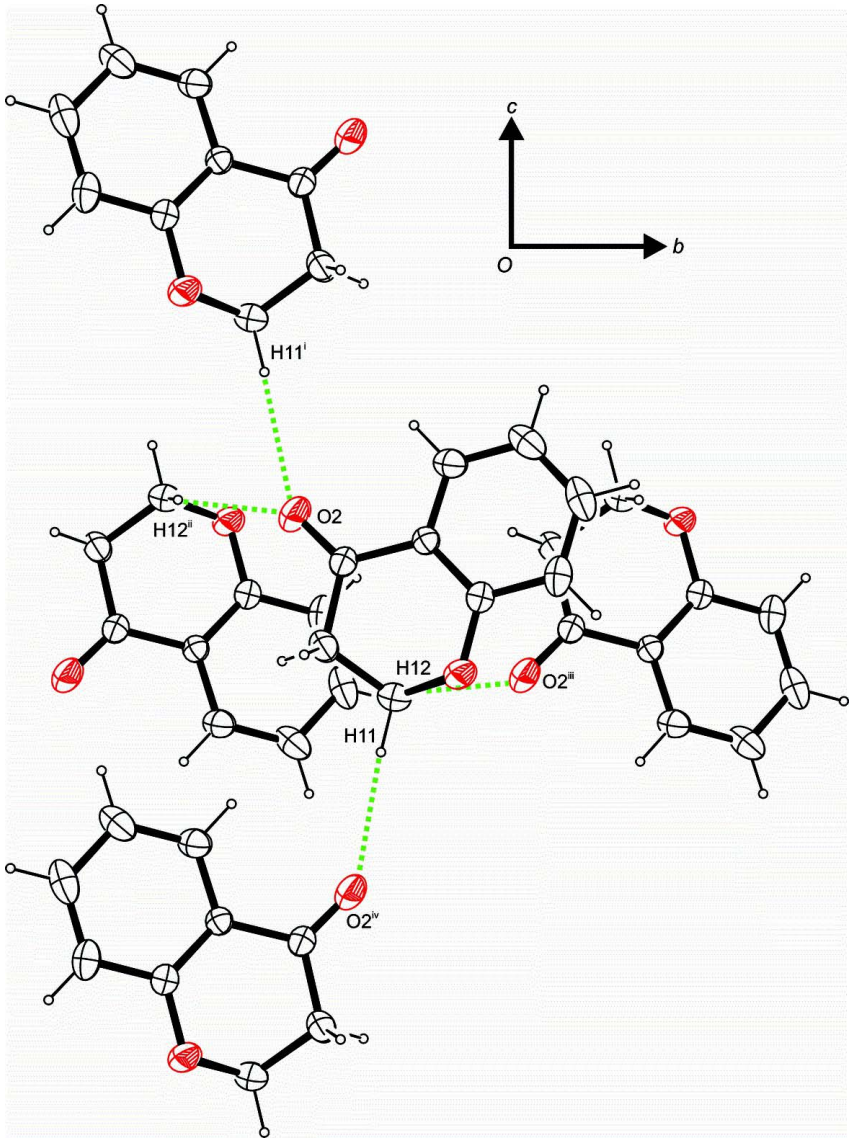

Figure 2

Intermolecular contacts, viewed along [-1 0 0]. Symmetry operators: [i] *x*, -*y* + 1/2, *z* + 1/2; [ii] -*x*, *y* - 1/2, -*z* + 1/2; [iii] -*x*, *y* + 1/2, -*z* + 1/2; [iv] *x*, -*y* + 1/2, *z* - 1/2.

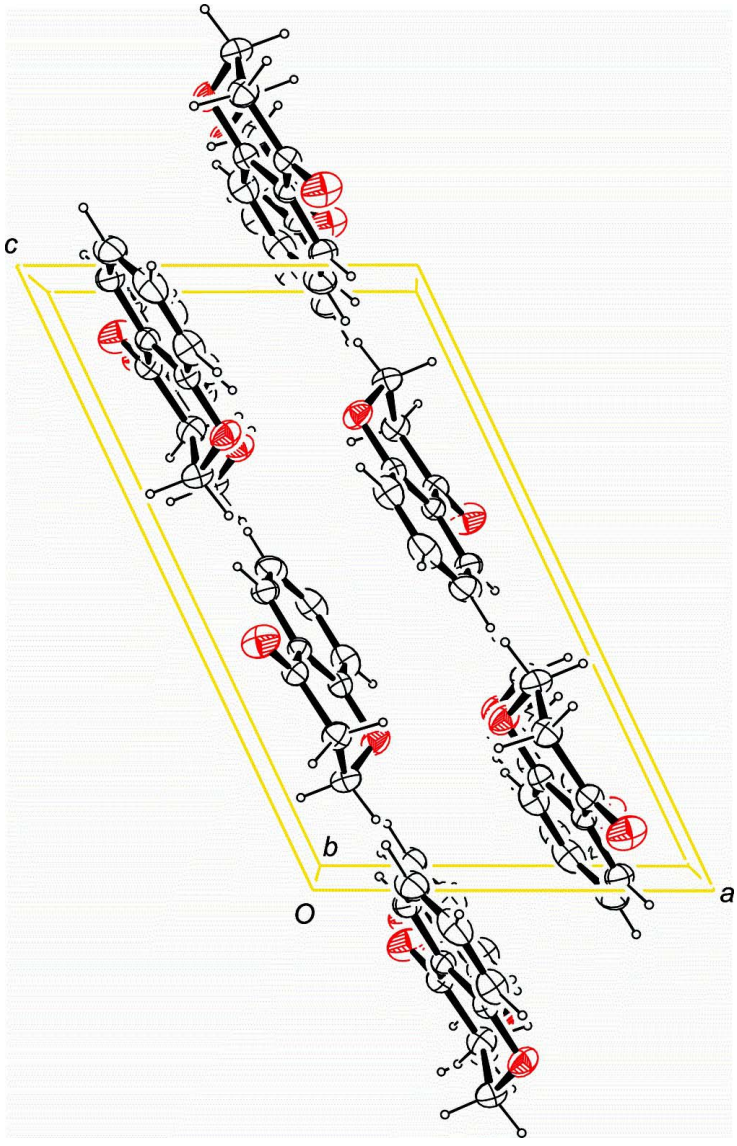

Figure 3

Molecular packing of the title compound, viewed along [0 1 0] (anisotropic displacement ellipsoids drawn at 50% probability level).

2*H*-Chromen-4(3*H*)-one

Crystal data

$C_9H_8O_2$
M_r = 148.15
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.5538 (4) Å
b = 8.0896 (4) Å
c = 13.0410 (6) Å
β = 115.364 (3)°
V = 720.08 (6) Å^3
Z = 4

$F(000)$ = 312
D_x = 1.367 Mg m^{-3}
Melting point = 308–311 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4401 reflections
θ = 3.0–28.3°
μ = 0.10 mm^{-1}
T = 200 K
Block, colourless
0.48 × 0.41 × 0.29 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
6367 measured reflections
1774 independent reflections
1578 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 28.3°$, $\theta_{min} = 3.5°$
$h = -9 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -17 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.107$
$S = 1.05$
1774 reflections
100 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.1339P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.32152 (11)	0.53935 (9)	0.22765 (6)	0.0337 (2)
O2	0.15764 (13)	0.19047 (10)	0.39707 (7)	0.0434 (2)
C1	0.20014 (15)	0.40212 (13)	0.16627 (8)	0.0327 (2)
H11	0.2296	0.3735	0.1014	0.039*
H12	0.0606	0.4348	0.1357	0.039*
C2	0.23447 (15)	0.25263 (12)	0.24191 (8)	0.0307 (2)
H21	0.1432	0.1632	0.1991	0.037*
H22	0.3699	0.2120	0.2654	0.037*
C3	0.20392 (13)	0.29406 (11)	0.34541 (8)	0.0262 (2)
C4	0.23848 (12)	0.46883 (11)	0.38176 (7)	0.0232 (2)
C5	0.29805 (12)	0.58227 (11)	0.32203 (8)	0.0255 (2)
C6	0.33856 (14)	0.74544 (12)	0.35963 (9)	0.0349 (2)
H6	0.3802	0.8228	0.3197	0.042*
C7	0.31759 (15)	0.79357 (13)	0.45538 (10)	0.0400 (3)
H7	0.3450	0.9047	0.4807	0.048*
C8	0.25740 (16)	0.68291 (14)	0.51532 (9)	0.0389 (3)
H8	0.2424	0.7180	0.5807	0.047*
C9	0.21953 (14)	0.52099 (13)	0.47876 (8)	0.0310 (2)
H9	0.1801	0.4441	0.5200	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0403 (4)	0.0338 (4)	0.0332 (4)	−0.0066 (3)	0.0217 (3)	0.0014 (3)
O2	0.0608 (5)	0.0309 (4)	0.0420 (4)	−0.0108 (3)	0.0254 (4)	0.0046 (3)
C1	0.0385 (5)	0.0353 (5)	0.0253 (4)	−0.0009 (4)	0.0146 (4)	−0.0024 (4)

C2	0.0348 (5)	0.0262 (4)	0.0318 (5)	−0.0008 (4)	0.0147 (4)	−0.0051 (4)
C3	0.0263 (4)	0.0239 (4)	0.0267 (4)	−0.0010 (3)	0.0098 (3)	0.0018 (3)
C4	0.0221 (4)	0.0233 (4)	0.0231 (4)	0.0013 (3)	0.0086 (3)	0.0007 (3)
C5	0.0234 (4)	0.0240 (4)	0.0279 (4)	−0.0001 (3)	0.0098 (3)	0.0012 (3)
C6	0.0318 (5)	0.0236 (5)	0.0446 (6)	−0.0032 (4)	0.0117 (4)	0.0013 (4)
C7	0.0329 (5)	0.0275 (5)	0.0474 (6)	0.0022 (4)	0.0057 (4)	−0.0114 (4)
C8	0.0374 (5)	0.0423 (6)	0.0314 (5)	0.0087 (4)	0.0095 (4)	−0.0107 (4)
C9	0.0313 (5)	0.0358 (5)	0.0256 (4)	0.0042 (4)	0.0121 (4)	0.0001 (4)

Geometric parameters (Å, º)

O1—C5	1.3616 (11)	C4—C5	1.3970 (12)
O1—C1	1.4439 (12)	C4—C9	1.3977 (13)
O2—C3	1.2166 (12)	C5—C6	1.3957 (13)
C1—C2	1.5112 (14)	C6—C7	1.3803 (16)
C1—H11	0.9900	C6—H6	0.9500
C1—H12	0.9900	C7—C8	1.3870 (18)
C2—C3	1.5013 (13)	C7—H7	0.9500
C2—H21	0.9900	C8—C9	1.3813 (15)
C2—H22	0.9900	C8—H8	0.9500
C3—C4	1.4785 (12)	C9—H9	0.9500
C5—O1—C1	113.55 (7)	C5—C4—C3	120.27 (8)
O1—C1—C2	111.27 (8)	C9—C4—C3	120.43 (9)
O1—C1—H11	109.4	O1—C5—C6	117.70 (9)
C2—C1—H11	109.4	O1—C5—C4	122.30 (8)
O1—C1—H12	109.4	C6—C5—C4	119.99 (9)
C2—C1—H12	109.4	C7—C6—C5	119.45 (10)
H11—C1—H12	108.0	C7—C6—H6	120.3
C3—C2—C1	111.02 (8)	C5—C6—H6	120.3
C3—C2—H21	109.4	C6—C7—C8	121.35 (9)
C1—C2—H21	109.4	C6—C7—H7	119.3
C3—C2—H22	109.4	C8—C7—H7	119.3
C1—C2—H22	109.4	C9—C8—C7	119.13 (10)
H21—C2—H22	108.0	C9—C8—H8	120.4
O2—C3—C4	122.29 (9)	C7—C8—H8	120.4
O2—C3—C2	122.37 (9)	C8—C9—C4	120.82 (10)
C4—C3—C2	115.33 (8)	C8—C9—H9	119.6
C5—C4—C9	119.25 (9)	C4—C9—H9	119.6
C5—O1—C1—C2	−55.93 (11)	C3—C4—C5—O1	1.80 (13)
O1—C1—C2—C3	55.36 (11)	C9—C4—C5—C6	0.23 (13)
C1—C2—C3—O2	154.40 (10)	C3—C4—C5—C6	−177.25 (8)
C1—C2—C3—C4	−26.96 (11)	O1—C5—C6—C7	−179.64 (9)
O2—C3—C4—C5	177.76 (9)	C4—C5—C6—C7	−0.55 (14)
C2—C3—C4—C5	−0.88 (12)	C5—C6—C7—C8	0.14 (15)
O2—C3—C4—C9	0.32 (14)	C6—C7—C8—C9	0.60 (16)
C2—C3—C4—C9	−178.33 (8)	C7—C8—C9—C4	−0.93 (15)

C1—O1—C5—C6	−153.72 (9)	C5—C4—C9—C8	0.52 (14)
C1—O1—C5—C4	27.22 (12)	C3—C4—C9—C8	177.99 (8)
C9—C4—C5—O1	179.27 (8)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H11···O2^{i}	0.99	2.53	3.4674 (13)	157
C1—H12···O2^{ii}	0.99	2.56	3.3934 (15)	141

Symmetry codes: (i) x, $-y+1/2$, $z-1/2$; (ii) $-x$, $y+1/2$, $-z+1/2$.