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2-(Diphenylmethylidene)-2,3-dihydro-1H-inden-1-one

Tao Zhang
Technological University Dublin, tao.zhang@tudublin.ie

Vilmar Bandero
Trinity College Dublin, Ireland

Tom McCabe
Trinity College Dublin, Ireland

Neil Frankish
Trinity College Dublin, Ireland

Helen Sheridan
Trinity College Dublin, Ireland

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2-(Diphenylmethylidene)-2,3-dihydro-1H-inden-1-one

Tao Zhang,* Vilmar Bandero,* Tom McCabe, Neil Frankish† and Helen Sheridan*‡

*Drug Discovery Group, School of Pharmacy and Pharmaceutical Sciences, Trinity College Dublin, Dublin 2, Ireland, and ‡School of Chemistry, Trinity College Dublin, Dublin 2, Ireland

Correspondence e-mail: hsheridn@tcd.ie

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Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.004 Å; R factor = 0.070; wR factor = 0.145; data-to-parameter ratio = 12.8.

In the title molecule, C22H16O, the indanone ring system is approximately planar with a dihedral angle between the fused rings of 51.3 (14)°. Two benzene rings are linked together at one side of a double bond, sitting on either side of the indanone ring system and making dihedral angles of 70.3 (12)° and 44.7 (13)° with it. In the crystal, hydrogen bonding is not present, but weak C–H · · ·π or π–π interactions occur and molecules form a sheet-like structure in the bc plane.

Related literature

For background to the indanone pharmacophore, its use as an organic intermediate and its biological activity, see: Buckle et al. (1973); Sheridan et al. (1990, 1999a,b, 2008, 2009a,b); Vacca et al. (1994); Schumann et al. (2001); Herzog et al. (2002); Frankish et al. (2004); Frankish & Sheridan (2012); Dinges et al. (2006); Kou et al. (2012); Ito et al. (2004); Jaki et al. (1999); Chanda et al. (2012); Chen et al. (2008); Rukachaisirikul et al. (2013); Farrell et al. (1996); Borbone et al. (2011); Fu & Wang (2008). For bond lengths and angles in related compounds, see: Ali et al. (2010a,b, 2011); Chen et al. (2011a, 2011b); Li et al. (2012); Lin et al. (2012).

Experimental

Crystal data

C22H16O

M(r) = 296.35

Monoclinic, P21/c

a = 9.1634 (18) Å

Experimental

Crystal data

C22H16O

M(r) = 296.35

Monoclinic, P21/c

a = 9.1634 (18) Å

b = 17.570 (3) Å

c = 10.717 (4) Å

β = 117.89 (2)°

V = 1525.0 (7) Å³

Z = 4

Mo Kα radiation

μ = 0.08 mm⁻¹

T = 150 K

0.50 × 0.20 × 0.20 mm

Data collection

Rigaku Saturn 724 diffractometer

Absorption correction: multi-scan (CrystalClear; Rigaku, 2006)

Tmin = 0.763, Tmax = 1.000

2680 independent reflections

Refinement

R[F² > 2σ(F²)] = 0.070

wR(F²) = 0.145

S = 1.25

209 parameters

H-atom parameters constrained

Δρmax = 0.19 e Å⁻³

Δρmin = −0.24 e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

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

Data collection: CrystalClear (Rigaku, 2006); cell refinement: CrystalClear; data reduction: CrystalClear; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012) and Mercury (Macrae et al., 2006); software used to prepare material for publication: SHELXL97 and Mercury (Macrae et al., 2006).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2117).

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2-(Diphenylmethylidene)-2,3-dihydro-1H-inden-1-one

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**Comment**

The indanone scaffold has been widely observed in the natural world (Jaki et al., 1999; Ito et al., 2004; Chen et al., 2008; Chanda et al., 2012; Rukachaisirikul et al., 2013). As organic intermediates, many indanone derivatives are used during chemical synthesis (Sheridan et al., 1990; Farrell et al., 1996; Sheridan et al., 1999a,b; Frankish et al., 2004; Borbone et al., 2011; Fu & Wang, 2008). Many studies show indanone pharmacophore is associated with a wide variety of biological properties such as: KDR kinase inhibition, mast cell stabilization, smooth muscle relaxation, antioxidation, and is used to target diseases such as cancer and Alzheimer's disease (Schumann et al., 2001; Herzog et al., 2002; Dinges et al., 2006; Sheridan et al., 2009a,b; Kou et al., 2012).

The asymmetric unit of the title molecule (I) is shown in Figure 1. It crystallizes in the non-chiral, monoclinic space group P2₁/c. The two benzene rings, C8—C13 and C1—C6 in the molecule lie above and below the C16—C21 plane, with the dihedral angles 70.30 (12)° and 44.74 (13)°, respectively. The torsion angles of these two benzene groups are [C14—C7—C8—C9] = 56.4 (3)° and [C14—C7—C6—C5] = 36.5 (4)°. The rest of the molecule is essentially planar.

The indanone fraction shows the normal values for this type of molecules (Ali et al., 2010a,b; Ali et al., 2011; Li et al., 2012; Lin et al., 2012), with the C20—C21—C16—C15 bond angle being 176.3 (2)° and the bond length of benzylic carbonyl functionality (C22—O1) 1.231 (3) Å. The double bond (C14=C7) is located at alpha position to the carbonyl group of the indanone ring, with the bond length being 1.362 (4) Å. The geometry around quaternary C7 can be considered as a planar triangle: C14—C7—C8 = 119.0 (2)°, C14—C7—C6 = 126.2 (3)° and C6—C7—C8 = 114.6 (2)°. The packing diagrams of the molecular structure are presented in Figure 2. Weak intermolecular C—H···π and π—π interactions are observed in Figure 2a, which seems to be very effective in the stabilization of the crystal structure. Figure 2b shows that the molecules are separated by forming a sheet-like structure in the bc-plane when viewed along the crystallographic b-axis. It is suggested that weak Van der Vaals force or electrostatic interaction could be contributed to the linkage of the sheets.

**Experimental**

To a stirred solution of 2-((2-hydroxyethoxy)diphenylmethyl)-2,3-dihydroinden-1-one (2.23 mmol) in methanol/DCM (12 ml, v:v, 3:1) was added trifluoromethanesulfonic acid (0.2 ml). The reaction was stirred at reflux for one hour, after which time the reaction was quenched by the addition of 2M NaOH aq. solution (20 ml) and the product was extracted with DCM (3 x 25 ml). The combined organic extracts were dried over magnesium sulfate, filtered and concentrated in vacuo, and the residue was purified by flash column chromatography on silica gel 230–400mesh (eluent: hexane: ethyl acetate, 10:1). All homogenous fractions were collected and the solvent removed in vacuo to afford titled crossed aldol condensed compound (94%) as yellow solid. Crystals suitable for X-ray diffraction were obtained after 7 days of slow evaporation of an ethyl acetate solution.
Refinement

All H atoms were placed in geometrically idealized positions and treated using the riding model, with C—H = 0.93–0.97 Å for H atoms. $U_{iso}(H)$ values were set at 1.2–1.5 times $U_{eq}(C)$ for the H atoms in the molecule.

Computing details

Data collection: CrystalClear (Rigaku, 2006); cell refinement: CrystalClear (Rigaku, 2006); data reduction: CrystalClear (Rigaku, 2006); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012) and Mercury (Macrae et al., 2006); software used to prepare material for publication: SHELXL97 (Sheldrick, 2008) and Mercury (Macrae et al., 2006).

Figure 1

The molecule structure of the titled compound with the atom numbering scheme. Displacement ellipsoids are shown at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.
Figure 2
a. The molecular packing, viewed along the $a$ axis.

Figure 3
b. The molecular packing, viewed along the $b$ axis.

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Crystal data

\begin{align*}
C_{22}H_{16}O & \quad \beta = 117.89 (2)^\circ \\
M_r = 296.35 & \quad V = 1525.0 (7) \text{ Å}^3 \\
Monoclinic, \ P_{2_1}/c & \quad Z = 4 \\
Hall symbol: -P\ 2ybc & \quad F(000) = 624 \\
a = 9.1634 (18) \text{ Å} & \quad D_a = 1.291 \text{ Mg m}^{-3} \\
b = 17.570 (3) \text{ Å} & \quad \text{Mo } K\alpha \text{ radiation, } \lambda = 0.71073 \text{ Å} \\
c = 10.717 (4) \text{ Å} & \quad \text{Cell parameters from 5979 reflections}
\end{align*}
θ = 2.4–31.1°
μ = 0.08 mm⁻¹
T = 150 K

**Data collection**

Rigaku Saturn 724
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan
(CrystalClear; Rigaku, 2006)
O.50 × 0.20 × 0.20 mm

Prism, colourless

2680 independent reflections
2587 reflections with I > 2σ(I)
θmax = 25.0°, θmin = 2.4°
h = −10→10
k = −20→13
l = −11→12

4590 standard reflections every 120 reflections

**Refinement**

Refinement on F²
Least-squares matrix: full
R[F² > 2σ(F²)] = 0.070
wR(F²) = 0.145
S = 1.25
2680 reflections
209 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

Δρmax = 0.19 e Å⁻³
Δρmin = −0.24 e Å⁻³

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

| x     | y     | z     | Uiso*/Ueq |
|-------|-------|-------|-----------|
| O1    | 0.3991 (2) | 0.62562 (11) | 0.58262 (19) | 0.0266 (4) |
| C1    | 0.2609 (3) | 0.69082 (14) | 0.1518 (3) | 0.0216 (6) |
| H1    | 0.1860 | 0.7305 | 0.1127 | 0.026* |
| C2    | 0.3856 (3) | 0.68115 (15) | 0.1133 (3) | 0.0241 (6) |
| H2    | 0.3944 | 0.7148 | 0.0502 | 0.029* |
| C3    | 0.4960 (3) | 0.62161 (15) | 0.1689 (3) | 0.0256 (6) |
| H3    | 0.5790 | 0.6151 | 0.1431 | 0.031* |
| C4    | 0.4829 (3) | 0.57117 (16) | 0.2640 (3) | 0.0253 (6) |
| H4    | 0.5567 | 0.5309 | 0.3009 | 0.030* |
| C5    | 0.3595 (3) | 0.58118 (15) | 0.3035 (3) | 0.0230 (6) |
| H5    | 0.3517 | 0.5475 | 0.3671 | 0.028* |
| C6    | 0.2469 (3) | 0.64149 (14) | 0.2488 (3) | 0.0200 (5) |
| C7    | 0.1051 (3) | 0.65032 (13) | 0.2802 (3) | 0.0192 (5) |
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|   | U \(^1\)    | U \(^2\)    | U \(^3\)    | U \(^12\) | U \(^13\) | U \(^23\) |
|---|------------|------------|------------|----------|----------|----------|
| O1| 0.0225 (10)| 0.0323 (11)| 0.0230 (10)| −0.0011 (8)| 0.0091 (8)| 0.0002 (8)|
| C1| 0.0214 (13)| 0.0210 (13)| 0.0214 (14)| −0.0001 (10)| 0.0091 (11)| −0.0005 (10)|
| C2| 0.0263 (14)| 0.0235 (14)| 0.0240 (15)| −0.0064 (11)| 0.0130 (12)| −0.0018 (11)|
| C3| 0.0200 (13)| 0.0327 (15)| 0.0256 (15)| −0.0035 (11)| 0.0119 (12)| −0.0076 (12)|
| C4| 0.0204 (13)| 0.0296 (14)| 0.0231 (15)| 0.0028 (11)| 0.0079 (12)| −0.0016 (11)|
| C5| 0.0236 (13)| 0.0230 (13)| 0.0213 (14)| 0.0013 (10)| 0.0095 (12)| 0.0026 (10)|
| C6| 0.0197 (12)| 0.0198 (12)| 0.0184 (13)| −0.0034 (10)| 0.0072 (11)| −0.0041 (10)|
| C7| 0.0197 (13)| 0.0159 (12)| 0.0209 (14)| −0.0008 (10)| 0.0087 (11)| −0.0019 (10)|
| C8| 0.0191 (13)| 0.0194 (12)| 0.0206 (14)| −0.0003 (10)| 0.0099 (11)| 0.0045 (10)|
| C9| 0.0246 (13)| 0.0233 (13)| 0.0289 (15)| 0.0012 (11)| 0.0155 (12)| 0.0057 (11)|
| C10| 0.0228 (14)| 0.0286 (15)| 0.0444 (19)| 0.0074 (12)| 0.0191 (14)| 0.0168 (13)|
| C11| 0.0203 (13)| 0.0411 (17)| 0.0319 (17)| 0.0016 (12)| 0.0077 (13)| 0.0205 (14)|
| C12| 0.0267 (15)| 0.0394 (17)| 0.0192 (15)| −0.0054 (12)| 0.0059 (12)| 0.0053 (12)|
| C13| 0.0236 (14)| 0.0301 (14)| 0.0220 (15)| 0.0011 (11)| 0.0101 (12)| 0.0041 (11)|
| C14| 0.0211 (13)| 0.0175 (12)| 0.0201 (14)| −0.0005 (10)| 0.0099 (11)| −0.0005 (10)|
| C15| 0.0221 (13)| 0.0251 (13)| 0.0220 (14)| 0.0017 (11)| 0.0112 (11)| 0.0021 (11)|
| C16| 0.0280 (14)| 0.0149 (12)| 0.0205 (14)| −0.0005 (10)| 0.0122 (12)| −0.0030 (10)|
| C17| 0.0266 (14)| 0.0209 (13)| 0.0276 (15)| −0.0029 (11)| 0.0156 (12)| −0.0037 (11)|
| C18| 0.0378 (16)| 0.0229 (13)| 0.0257 (15)| −0.0037 (12)| 0.0197 (13)| −0.0021 (11)|
| C19| 0.0378 (16)| 0.0260 (14)| 0.0188 (14)| −0.0049 (12)| 0.0125 (13)| −0.0010 (11)|

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|          |          |          |          |          |          |          |
|----------|----------|----------|----------|----------|----------|----------|
| C20      | 0.0280 (14) | 0.0224 (13) | 0.0219 (14) | −0.0072 (11) | 0.0094 (12) | −0.0052 (11) |
| C21      | 0.0269 (14) | 0.0158 (12) | 0.0219 (14) | −0.0021 (10) | 0.0130 (12) | −0.0033 (10) |
| C22      | 0.0233 (14) | 0.0168 (12) | 0.0229 (14) | −0.0011 (10) | 0.0119 (12) | −0.0029 (10) |

Geometric parameters (Å, °)

| Bond  | Length (Å) | Angle (°)  |
|-------|------------|------------|
| O1—C22 | 1.231 (3) | C11—C12 1.389 (4) |
| C1—C2  | 1.395 (3) | C11—H11 0.9300 |
| C1—C6  | 1.405 (3) | C12—C13 1.388 (4) |
| C1—H1  | 0.9300 | C12—H12 0.9300 |
| C2—C3  | 1.382 (4) | C13—H13 0.9300 |
| C2—H2  | 0.9300 | C14—C22 1.501 (4) |
| C3—C4  | 1.397 (4) | C14—C15 1.525 (3) |
| C3—H3  | 0.9300 | C15—C16 1.508 (3) |
| C4—C5  | 1.392 (4) | C15—H15A 0.9700 |
| C4—H4  | 0.9300 | C15—H15B 0.9700 |
| C5—C6  | 1.402 (4) | C16—C17 1.393 (4) |
| C5—H5  | 0.9300 | C16—C21 1.397 (4) |
| C6—C7  | 1.495 (3) | C17—C18 1.388 (4) |
| C7—C14 | 1.362 (4) | C17—H17 0.9300 |
| C7—C8  | 1.498 (3) | C18—C19 1.403 (4) |
| C8—C13 | 1.398 (4) | C18—H18 0.9300 |
| C8—C9  | 1.404 (4) | C19—C20 1.396 (4) |
| C9—C10 | 1.394 (4) | C19—H19 0.9300 |
| C9—H9  | 0.9300 | C20—C21 1.402 (4) |
| C10—C11| 1.391 (4) | C20—H20 0.9300 |
| C10—H10| 0.9300 | C21—C22 1.488 (3) |

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C13—C8—C7 120.4 (2) C20—C19—C18 120.0 (3)
C9—C8—C7 121.0 (2) C20—C19—H19 120.0
C10—C9—C8 120.4 (3) C18—C19—H19 120.0
C10—C9—H9 119.8 C19—C20—C21 118.1 (2)
C8—C9—C7 121.0 (2) C19—C20—H20 120.9
C11—C10—C9 120.0 (3) C21—C20—H20 120.9
C11—C10—H10 120.0 C16—C21—C20 121.5 (2)
C9—C10—H10 120.0 C16—C21—C22 109.9 (2)
C12—C11—C10 120.2 (3) C20—C21—C22 128.6 (2)
C12—C11—H11 119.9 O1—C22—C21 125.0 (2)
C10—C11—H11 119.9 O1—C22—C14 128.5 (2)
C13—C12—C11 119.8 (3) C21—C22—C14 106.5 (2)
C13—C12—H12 120.1

C6—C1—C2—C3 1.1 (4) C1—C6—C7—C14 163.5 (2)
C1—C2—C3—C4 −0.1 (4) C8—C7—C14—C15 10.9 (4)
C2—C3—C4—C5 −0.5 (4) C7—C14—C15—C16 170.5 (2)
C3—C4—C5—C6 0.2 (4) C22—C14—C15—C16 −6.8 (3)
C4—C5—C6—C1 0.7 (4) C14—C15—C16—C17 −174.2 (2)
C4—C5—C6—C7 175.1 (2) C16—C17—C18—C19 0.5 (4)
C2—C1—C6—C5 −1.4 (4) C21—C16—C17—C18 −178.1 (2)
C2—C1—C6—C7 −175.9 (2) C15—C16—C17—C18 −178.1 (2)
C5—C6—C7—C14 36.5 (4) C16—C17—C18—C19 1.8 (4)
C6—C7—C8—C13 149.2 (3) C17—C18—C19—C20 −2.0 (4)
C5—C6—C7—C8 −138.0 (2) C18—C19—C20—C21 0.0 (4)
C1—C6—C7—C8 36.2 (3) C17—C16—C21—C20 −2.5 (4)
C14—C7—C8—C13 −123.9 (3) C15—C16—C21—C20 176.3 (2)
C6—C7—C8—C9 51.1 (3) C17—C16—C21—C22 176.4 (2)
C14—C7—C8—C9 56.4 (3) C15—C16—C21—C22 −4.8 (3)
C6—C7—C8—C13 −128.6 (2) C19—C20—C21—C16 2.2 (4)
C13—C8—C9—C10 2.1 (4) C19—C20—C21—C22 −176.5 (2)
C7—C8—C9—C10 −178.2 (2) C16—C21—C22—O1 178.9 (2)
C8—C9—C10—C11 −0.2 (4) C20—C21—C22—O1 −2.2 (4)
C9—C10—C11—C12 −0.9 (4) C16—C21—C22—C14 0.2 (3)
C10—C11—C12—C13 0.1 (4) C20—C21—C22—C14 179.1 (2)
C11—C12—C13—C8 1.9 (4) C7—C14—C22—C14 8.6 (4)
C9—C8—C13—C12 −2.9 (4) C15—C14—C22—C14 −174.4 (2)
C7—C8—C13—C12 177.3 (2) C7—C14—C22—C21 −172.8 (2)
C6—C7—C14—C22 13.2 (4) C15—C14—C22—C21 4.2 (3)
C8—C7—C14—C22 −172.5 (2)

Hydrogen-bond geometry (Å, °)
Cg1, Cg2 and Cg4 are the centroids of the C14–C16/C21/C22, C1–C6 and C16–C21 rings, respectively.

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|--------|
| C1—H1···Cg1i | 0.93 | 2.91 | 3.763 (3) | 153 |
| C11—H11···Cg2ii | 0.93 | 2.99 | 3.712 (3) | 136 |
| C15—H15B···Cg4iii | 0.97 | 2.92 | 3.640 (3) | 132 |

Symmetry codes: (i) x, −y+3/2, z−1/2; (ii) x−1, −y+3/2, z−1/2; (iii) −x, −y+1, −z+1.

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