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Spiro[1,1a,6,6a-Tetrahydrocyclopropa[*a*]indene-1,1′-2′,3′-dihydro-1′*H*-indene]

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.140
Data-to-parameter ratio = 18.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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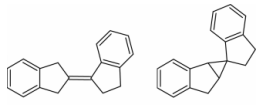
In the crystal structure of the title compound, $C_{18}H_{16}$, the two nearly planar halves of the molecule [maximum deviations from planarity 0.0324 (13) and 0.0441 (11) Å] are connected *via* two C—C bonds which are formed between one C atom in the five-membered ring of one half and two neighbouring C atoms in the five-membered ring of the other half, forming a central three-membered C ring with C—C distances between the rings of 1.5321 (19) and 1.5040 (18) Å. The dihedral angle between the least-squares planes through the non-H atoms of the molecule halves is 86.56 (3)°.

Comment

In the course of our investigations on the four possible biindenylidene isomers, we have already reported a second modification of (*E*)-2,3,2′,3′-tetrahydro-[1,1′]biindenylidene (Jovanovic *et al.*, 2001*a*) and the crystal structure of 1,3,1′,3′-tetrahydro-[2,2′]biindenylidene (Jovanovic *et al.*, 2001*b*). We wished next to determine the crystal structure of 2,3,1′,3′-tetrahydro-[1,2′]-biindenylidene, (I), and synthesized it following the description of Bell & Spanswick (1966). The compound we obtained had the same melting point and molecular weight as previously reported for the structure (I), but our crystallographic investigations show that it actually has the structure (II).



(I) (II)

Experimental

Spiro[1,1a,6,6a-tetrahydro-cyclopropa[*a*]indene-1,1′-2′,3′-dihydro-1′*H*-indene] was synthesized through the aldol condensation of 1*H*-indan-1-one and the Huang–Minlon reduction of the self-condensation product according to the method of Bell & Spanswick (1966). It was isolated by crystallization from propan-2-ol.

Crystal data

$C_{18}H_{16}$
M_r = 232.31
Monoclinic, $P2_1/c$
a = 7.0256 (1) Å
b = 12.5288 (2) Å
c = 14.8003 (4) Å
β = 94.3527 (9)°
V = 1299.00 (4) Å^3
Z = 4
D_x = 1.188 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 13022 reflections
θ = 3.2–27.5°
μ = 0.07 mm^{-1}
T = 291 (1) K
Block, colourless
0.48 × 0.45 × 0.15 mm

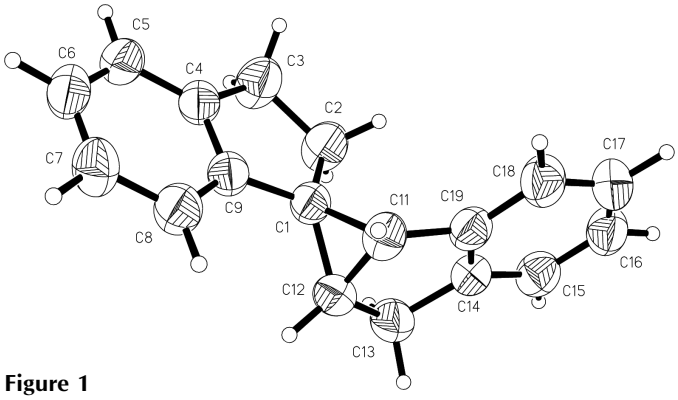


Figure 1
View of the title compound (*XP*; Sheldrick, 1991) showing the labelling of all non-H atoms. Displacement ellipsoids are shown at the 50% probability level.

Data collection

Nonius KappaCCD diffractometer
318 frames *via* ω-rotation ($\Delta\omega = 1^\circ$) with 3 sets at different κ-angles and two times 60 s per frame
Absorption correction: none
13022 measured reflections
2965 independent reflections

1842 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.5^\circ$
$h = -9 \rightarrow 9$
$k = -16 \rightarrow 16$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.140$
$S = 1.07$
2965 reflections
163 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0785P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

H atoms were placed in calculated positions with U_{iso} constrained to be 1.2 times U_{eq} of the carrier atom.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97, *PARST*95 (Nardelli, 1995) and *PLATON* (Spek, 2001).

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