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1,3,1′,3′-Tetrahydro-[2,2′]biindenylidene

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.101
Data-to-parameter ratio = 17.5

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

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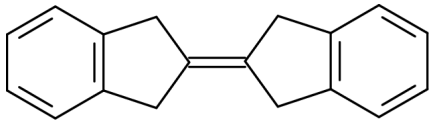
In the investigated crystal of the title compound, $C_{18}H_{16}$, the unit cell contains two centrosymmetric and nearly planar molecules [maximum deviation from planarity 0.0401 (10) Å]. The length of the central double bond is 1.322 (2) Å.

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). The crystal structure of the title compound, (I), has not been reported up to now. Biindenylidenes are components of many pyrolysis oils and their characterization is important in environmental analysis. They also represent useful model substances for MS and NMR analysis, and structural data are important for the understanding of some fine details of MS and NMR spectra.



(I)

Experimental

1,3,1′,3′-Tetrahydro-[2,2′]biindenylidene was synthesized and crystallized following the method described by Czogalla & Boberg (1987) by reductive coupling of 1*H*-indan-2-one.

Crystal data

$C_{18}H_{16}$
M_r = 232.31
Monoclinic, $P2_1/c$
a = 7.5489 (2) Å
b = 4.8968 (2) Å
c = 17.0874 (6) Å
β = 93.8964 (19)°
V = 630.18 (4) Å^3
Z = 2
D_x = 1.224 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5614 reflections
θ = 4.8–27.5°
μ = 0.07 mm^{-1}
T = 291 (1) K
Needle, colourless
0.30 × 0.07 × 0.07 mm

Data collection

Nonius KappaCCD diffractometer
284 frames *via* ω rotation ($\Delta\omega$ = 1°) with three sets at different κ angles and two times 100 s per frame
5614 measured reflections
1439 independent reflections
896 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.5°
$h = -9 \rightarrow 9$
$k = -6 \rightarrow 6$
$l = -22 \rightarrow 22$

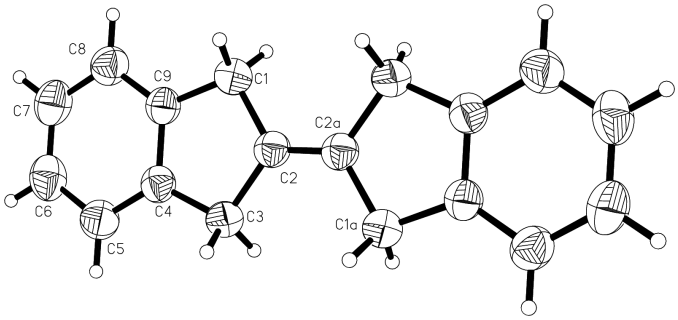


Figure 1
View of the title compound (*XP*; Sheldrick, 1991) showing the labelling of non-H atoms. The molecule is centrosymmetric. Displacement ellipsoids are shown at the 50% probability level. H atoms are drawn as circles of arbitrary radius.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.101$
$S = 0.90$
1439 reflections
82 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ 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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