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2-(2′,3′-Dihydro-1′*H*-inden1′-yl)-1*H*-indene

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.036
wR factor = 0.076
Data-to-parameter ratio = 7.9

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

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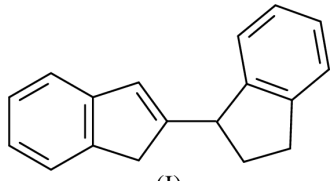
The dihedral angle between the least-squares planes through the C atoms of the six-membered rings of the title indene dimer, $C_{18}H_{16}$, is 85.53 (11)°. The five-membered ring in the indene moiety is nearly planar [torsion angles: −0.4 (3), 0.1 (4), 0.3 (4), −0.6 (3) and 0.6 (3)°], whereas the other five-membered ring deviates markedly from planarity [torsion angles: −15.3 (4), 14.3 (4), −7.8 (4), −1.5 (4), 10.7 (4)°]. The central C—C bond length is 1.488 (4) Å.

Comment

The title compound, (I), represents the most stable dimer of indene obtained by the cationic dimerization through the reaction of the 2,3-dihydro-1*H*-inden-1-yl carbenium ion with 1*H*-indene at position 2. Compound (I) was described in the literature by Moglioni *et al.* (1998) and Noland *et al.* (1979), but a crystal structure has not been reported previously. It is the constituent of many pyrolysis oils and its characterization is important for environmental analysis. It also represents a useful model substance for MS and NMR analysis, and structural data are important for the understanding of some fine details of MS and NMR spectra.



(I)

Experimental

The general procedure was the one described by Dansi & Pasini (1951). 10 g of indene (>99.0% purity) and 40 ml 48% H_2SO_4, as a two-phase mixture, were refluxed (oil-bath temperature 398–403 K) with vigorous stirring for 8 h. After cooling to room temperature, 100 ml cyclohexane were added. The reaction mixture was neutralized with $NaHCO_3$ (5%), washed with water and dried over Na_2SO_4. After evaporating the cyclohexane, 8.7 g of yellow viscous oil were obtained. It contained more than 85% of (I), which was isolated by crystallization from propan-2-ol.

Crystal data

$C_{18}H_{16}$
M_r = 232.31
Orthorhombic, *Fdd*2
a = 20.2837 (8) Å
b = 42.098 (2) Å
c = 6.1644 (2) Å
V = 5263.8 (4) Å^3
Z = 16
D_x = 1.173 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 10913 reflections
θ = 3.5–25.3°
μ = 0.07 mm^{-1}
T = 293 (1) K
Needle, colourless
0.50 × 0.05 × 0.02 mm

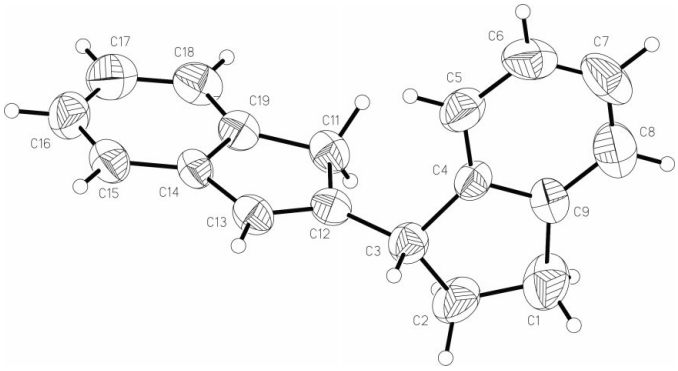


Figure 1
View of the title compound (*XP*; Sheldrick, 1991) showing the labelling of all non-H atoms. Displacement ellipsoids are shown at the 30% probability levels. H atoms are drawn as circles of arbitrary radii.

Data collection

Nonius KappaCCD diffractometer
319 frames *via* ω-rotation ($\Delta\omega = 1^\circ$) with 3 sets at different κ-angles and two times 150 s per frame
Absorption correction: none
10913 measured reflections
1285 independent reflections
565 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 25.3^\circ$
$h = -23 \rightarrow 23$
$k = -50 \rightarrow 50$
$l = -7 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.076$
$S = 0.82$
1285 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.10$ e Å^{-3}
$\Delta\rho_{min} = -0.10$ 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. Friedel opposites were merged and no attempt was made to refine the absolute configuration.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* 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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