Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*Z*)-2,3,2′,3′-Tetrahydro-[1,1′]biindenylidene

Jovan Jovanovic,[a] Wilhelm Elling,[b] Markus Schürmann,[c] Hans Preut[c]* and Michael Spiteller[b]

[a]Faculty of Technology and Metallurgy, University of Belgrade, PO Box 3503, 11120 Belgrade, Yugoslavia, [b]Institut für Umweltforschung, Universität Dortmund, Otto-Hahn-Str. 6, 44221 Dortmund, Germany, and [c]Fachbereich Chemie, Universität Dortmund, Otto-Hahn-Str. 6, 44221 Dortmund, Germany

Correspondence e-mail: uch002@uxp1.hrz.uni-dortmund.de

Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.042
wR factor = 0.111
Data-to-parameter ratio = 18.0

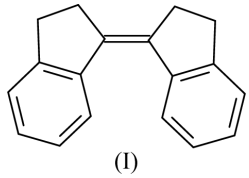
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 28 November 2001
Accepted 6 December 2001
Online 14 December 2001

The asymmetric unit in the crystal of the title compound, $C_{18}H_{16}$, contains two molecules with slightly different conformations. The dihedral angles between the least-squares planes through the C atoms of the phenyl rings in the two molecules are 25.89 (4) and 33.87 (4)°.

Comment

In the course of our investigations on the four possible biindenylidene isomers we 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*). The title compound, (I) (Fig. 1), has not been described previously in the literature. 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

The title compound was obtained from the reaction mixture that contained also *trans* isomer, *i.e.* (*E*)-2,3,2′,3′-tetrahydro-[1,1′]-biindenylidene, by two-step chromatography using column chromatography in the first and HPLC in the second step. The reaction mixture was obtained through the reductive coupling of 1*H*-indan-1-one according to the method of Lenoir & Lemmen (1980). Recrystallization from propan-2-ol gave colourless plates (m.p. 328 K).

Crystal data

$C_{18}H_{16}$
M_r = 232.31
Orthorhombic, *Pbca*
a = 14.7176 (2) Å
b = 14.7680 (2) Å
c = 23.5860 (3) Å
V = 5126.41 (12) Å^3
Z = 16
D_x = 1.204 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 14231 reflections
θ = 3.1–27.5°
μ = 0.07 mm^{-1}
T = 291 (1) K
Block, colourless
0.50 × 0.30 × 0.30 mm

Data collection

Nonius KappaCCD diffractometer	3134 reflections with $I > 2\sigma(I)$
357 frames *via* ω-rotation ($\Delta\omega = 1^\circ$) with 3 sets at different κ-angles and two times 60 s per frame	$R_{int} = 0.036$
	$\theta_{max} = 27.5^\circ$
	$h = -19 \rightarrow 19$
Absorption correction: none	$k = -19 \rightarrow 19$
14231 measured reflections	$l = -30 \rightarrow 30$
5855 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.061P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.111$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.91$	$\Delta\rho_{max} = 0.14$ e Å^{-3}
5855 reflections	$\Delta\rho_{min} = -0.13$ e Å^{-3}
325 parameters	

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* 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).

We thank the Alexander von Humboldt Foundation, Bonn, Germany for supporting the work in this paper through a fellowship to JJ. This article is dedicated to Professor Gerhard Spiteller on the occasion of his 70th birthday.

References

Jovanovic, J., Schürmann, M., Preut, H. & Spiteller, M. (2001*a*). *Acta Cryst.* E**57**, o1100–o1101.
Jovanovic, J., Schürmann, M., Preut, H. & Spiteller, M. (2001*b*). *Acta Cryst.* E**57**, o1139–o1140.
Lenoir, D. & Lemmen, P. (1980). *Chem. Ber.* **113**, 3112–3119.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter & R. M. Sweet, pp. 307–326. London: Academic Press.

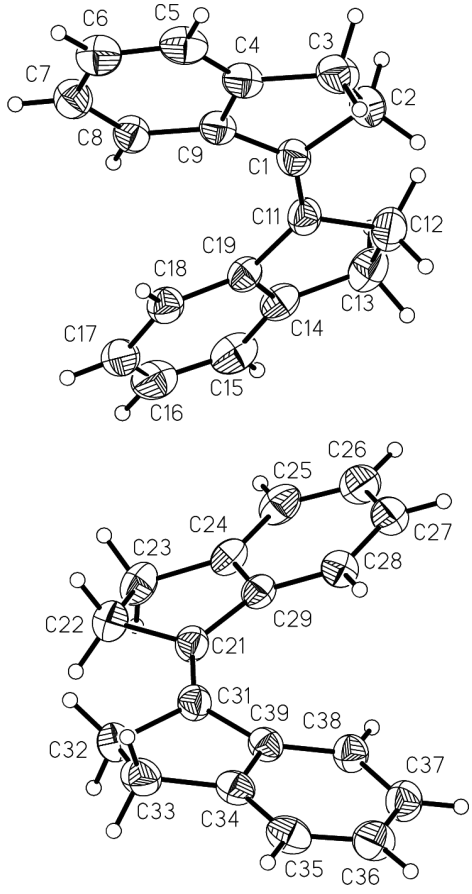


Figure 1
View of the title compound (*XP*; Sheldrick, 1991) showing the labelling of all non-H atoms. Displacement ellipsoids are shown at the 30% probability level. H atoms are drawn as circles of arbitrary radii.

Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1991). *SHELXTL-Plus.* Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2001). *PLATON.* University of Utrecht, The Netherlands.