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## Key indicators

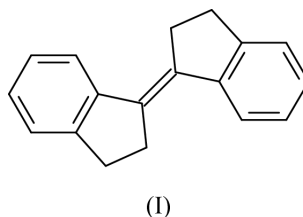
Single-crystal X-ray study  
T = 291 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
R factor = 0.050  
wR factor = 0.097  
Data-to-parameter ratio = 17.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Second modification of (*E*)-2,3,2',3'-tetrahydro-[1,1']-biindenylidene

A first crystalline modification of the title compound, C<sub>18</sub>H<sub>16</sub>, was published by Schaefer & Abulū [*Acta Cryst.* (1995), C51, 2364–2366]. We now report on a second modification. Both modifications belong to the space group *C2/c* and, in both, the molecules lie on centres of symmetry. In the first modification, the asymmetric unit contains one half molecule, whereas in the second there are two half-molecules in the asymmetric unit. The two crystallographically independent planar molecules of the second modification are tilted by an angle of 63.4° with respect to one another.

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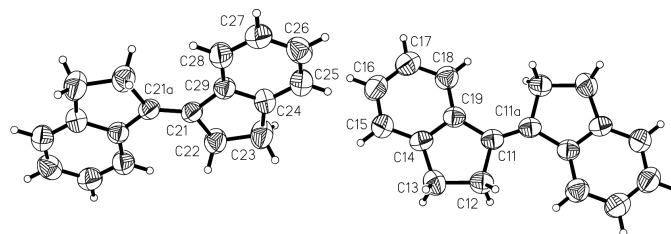
## Comment

(*E*)-2,3,2',3'-Tetrahydro-[1,1']biindenylidene, (I), is one of four possible biindenylidene isomers and the constituent of many pyrolysis oils. Its characterization is interesting 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.



## Experimental

(*E*)-2,3,2',3'-Tetrahydro-[1,1']biindenylidene was synthesized through the reductive coupling of 1*H*-indan-1-one according to the method of Lenoir & Lemmen (1980). It was isolated by crystallization from propan-2-ol.



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

*Crystal data*

C<sub>18</sub>H<sub>16</sub>  
*M<sub>r</sub>* = 232.31  
 Monoclinic, C2/c  
*a* = 43.717 (5) Å  
*b* = 8.0751 (10) Å  
*c* = 7.2651 (12) Å  
 $\beta$  = 96.860 (6)°  
*V* = 2546.4 (6) Å<sup>3</sup>  
*Z* = 8

*D<sub>x</sub>* = 1.212 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 7904 reflections  
 $\theta$  = 3.5–27.5°  
 $\mu$  = 0.07 mm<sup>-1</sup>  
*T* = 291 (1) K  
 Plate, light yellow  
 0.50 × 0.20 × 0.08 mm

*Data collection*

Nonius KappaCCD diffractometer  
 588 frames via  $\omega$ -rotation ( $\Delta\omega$  = 0.5%) and two times 20 s per frame (three sets at different  $\kappa$ -angles)  
 Absorption correction: none  
 2826 measured reflections

2826 independent reflections  
 780 reflections with  $I > \sigma(I)$   
 $R_{\text{int}} = 0.024$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -55 \rightarrow 55$   
 $k = -10 \rightarrow 10$   
 $l = -9 \rightarrow 9$

*Refinement*

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.050$   
 $wR(F^2) = 0.097$   
 $S = 0.83$   
 2826 reflections  
 163 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.015P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$

H atoms were placed in calculated positions with  $U_{\text{iso}}$  constrained to be 1.2 times  $U_{\text{eq}}$  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: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*, *PARST95* (Nardelli, 1995) and *PLATON* (Spek, 2001).

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**References**

- 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 and R. M. Sweet, pp. 307–326. London: Academic Press.  
 Schaefer, W. P. & Abulū, J. (1995). *Acta Cryst.* **C51**, 2364–2366.  
 Sheldrick, G. M. (1990). *Acta Cryst.* **A46**, 467–473.  
 Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.  
 Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.  
 Spek, A. L. (2001). *PLATON*. University of Utrecht, The Netherlands.