Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Spiro[cyclopropane-1,1′-1*H*-inden]-2′(3′*H*)-one

Jari Yli-Kauhaluoma,[b] Anja Salakari[c]* and Ilpo Mutikainen[a]

[a]University of Helsinki, Department of Chemistry, Laboratory of Inorganic Chemistry, FIN-00014 Helsinki, Finland, [b]University of Helsinki, Division of Pharmaceutical Chemistry, Faculty of Pharmacy, PO Box 56, FIN-00014 Helsinki, Finland, and [c]Technical Research Centre of Finland, VTT Processes, Industrial Chemistry, PO Box 1600, FI-02044 VTT, Finland

Correspondence e-mail:
ilpo.mutikainen@helsinki.fi

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.138
Data-to-parameter ratio = 12.7

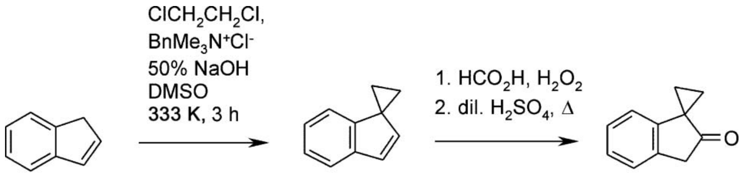
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 9 May 2006
Accepted 12 May 2006

The title compound, $C_{11}H_9O$, was prepared in two steps starting from indene. There are two crystallographically independent molecules in the asymmetric unit. Each is essentially planar, with only the atoms of the cyclopropanone group lying out of the molecular plane.

Comment

Recently, we have synthesized a plethora of spiro derivatives of both 1- and 2-indanone. Our attention was caught by their extraordinary structures (Baierweck *et al.*, 1985). We determined the X-ray crystallographic structure of the title compound, (I), in order to confirm the relative orientation of the three- and five-membered rings of the spiro system. There are two crystallographically independent molecules in the asymmetric unit. The molecules are essentally planar, with only the C and H atoms of the cyclopropanone groups connected to atoms C10*A* and C10*B* of the five-membered rings lying out of the molecular planes. The angle between the three- and five- membered rings in both molecules is exactly 90°.



(I)

Experimental

The title compound was conveniently prepared in two steps starting from indene (12.0 g, 0.103 mol). First, indene was allowed to react with 1,2-dibromoethane (13.4 ml, 0.155 mol) in the presence of benzyltrimethylammonium chloride (0.544 g, 2.93 mol) as a phase-transfer catalyst in 50% aqueous sodium hydroxide (48 ml) and dimethyl sulfoxide (20 ml) at 333 K for 3 h to give spiro[cyclopropane-1,1′-[1*H*]indene]. The resulting spiroindene (4.95 g, 34.8 mmol) was subsequently treated with performic acid [a mixture of 80% formic acid (24.4 ml) and 30% hydrogen peroxide (4.9 ml)] and dilute sulfuric acid (7%, 105 ml, steam distillation) to give the spiro derivative of 2-indanone in 49% overall yield after purification on SiO_2 (Bartha *et al.*, 1986).

Crystal data

$C_{11}H_9O$
M_r = 157.18
Monoclinic, $P2_1/m$
a = 8.941 (1) Å
b = 6.996 (1) Å
c = 13.491 (2) Å
β = 97.34 (1)°
V = 837.0 (2) Å^3
Z = 4
D_x = 1.247 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 (2) K
Prism, colourless
0.30 × 0.30 × 0.25 mm

© 2006 International Union of Crystallography
All rights reserved

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.977$, $T_{\max} = 0.981$

4074 measured reflections
2000 independent reflections
1511 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.019$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.138$
$S = 1.03$
2000 reflections
158 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2 + 0.4406P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.33$ e Å^{-3}
$\Delta\rho_{\min} = -0.26$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.061 (14)

H atoms were introduced in calculated positions (C—H = 0.95 Å and $U_{\rm iso}$(H) =1.2$U_{\rm eq}$ of the carrier atom) and refined with fixed geometry with respect to their carrier atoms , except for C10*A*, C10*B*, C11*A* and C11*B*, for which the H atoms were located in a difference map and their coordinates refined freely.

Data collection: *COLLECT* (Nonius, 2002); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EVAL* (Nonius, 2002); program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL*.

We thank the National Technology Agency TEKES for financial support.

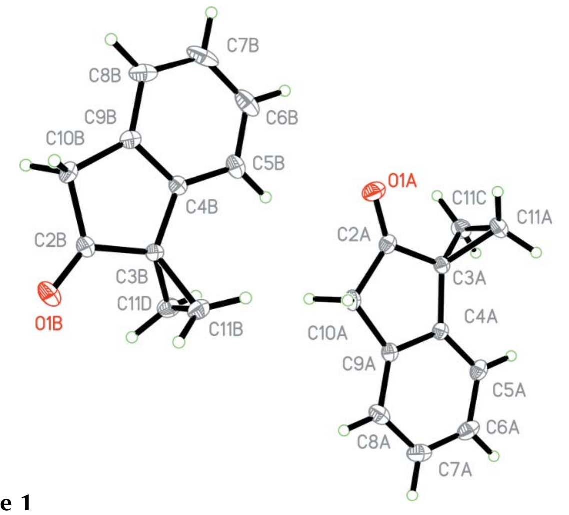


Figure 1
The asymmetric unit. Displacement ellipsoids are drawn at the 30% probability level.

References

Baierweck, P., Hoell, D. & Müllen, K. (1985). *Angew. Chem.* **97**, 959–960.
Bartha, E., Arvay, Z. & Razus, A. C. (1986). *Rev. Roum. Chim.* **31**, 519–524.
Burla, M. C., Camalli, M., Carrozzini, B., Casarano, G. L., Giacovazzo, C., Polidori, G. & Spagna, R. (2003). *J. Appl. Cryst.* **36**, 1103.
Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.
Nonius (2002). *COLLECT* and *EVAL*. Nonius BV, Delft, The Netherlands.
Sheldrick, G. M. (1990). *SHELXTL*. University of Göttingen, Germany.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

o2416 Mutikainen *et al.* • $C_{11}H_9O$ *Acta Cryst.* (2006). E**62**, o2415–o2416