C(21)	−0.0502 (3)	0.4196 (2)	0.3371 (2)	0.054 (1)
C(22)	0.0503 (3)	0.3760 (2)	0.3776 (2)	0.061 (1)
C(23)	0.1398 (4)	0.4290 (3)	0.4048 (2)	0.068 (2)
C(24)	0.1286 (4)	0.5255 (2)	0.3917 (2)	0.057 (1)
C(25)	−0.1234 (3)	0.9061 (2)	0.2470 (2)	0.041 (1)
C(26)	−0.0053 (3)	0.9420 (2)	0.1955 (2)	0.044 (1)
C(27)	0.1345 (4)	0.9345 (3)	0.2091 (2)	0.079 (2)
C(28)	0.2390 (5)	0.9726 (4)	0.1606 (2)	0.104 (2)
C(29)	0.2050 (6)	1.0182 (3)	0.0993 (2)	0.092 (2)
C(30)	0.0674 (6)	1.0248 (3)	0.0839 (2)	0.084 (2)
C(31)	−0.0385 (5)	0.9878 (3)	0.1321 (2)	0.067 (1)
O(1′)	−0.7344 (2)	0.2284 (2)	0.3441 (1)	0.066 (1)
O(2′)	−0.3330 (2)	0.4389 (2)	0.2401 (1)	0.064 (1)
C(1′)	−0.4211 (3)	0.4232 (2)	0.4063 (2)	0.049 (1)
C(2′)	−0.3435 (4)	0.4130 (2)	0.4624 (2)	0.057 (1)
C(3′)	−0.2706 (4)	0.3301 (2)	0.4843 (2)	0.053 (1)
C(4′)	−0.2730 (3)	0.2563 (2)	0.4499 (1)	0.043 (1)
C(4*A*′)	−0.3499 (3)	0.2666 (2)	0.3938 (1)	0.034 (1)
C(4*B*′)	−0.3646 (3)	0.1970 (2)	0.3482 (1)	0.032 (1)
C(4*C*′)	−0.2426 (3)	0.1956 (2)	0.2963 (1)	0.032 (1)
C(5′)	−0.1006 (3)	0.1829 (2)	0.3070 (2)	0.042 (1)
C(6′)	−0.0029 (3)	0.1877 (3)	0.2518 (2)	0.055 (1)
C(7′)	−0.0470 (3)	0.2083 (3)	0.1876 (2)	0.060 (1)
C(8′)	−0.1874 (3)	0.2206 (2)	0.1761 (2)	0.052 (1)
C(8*A*′)	−0.2870 (3)	0.2119 (2)	0.2314 (1)	0.035 (1)
C(9′)	−0.4425 (3)	0.2235 (2)	0.2334 (1)	0.033 (1)
C(9*A*′)	−0.4902 (3)	0.2369 (2)	0.3049 (1)	0.031 (1)
C(10′)	−0.5057 (3)	0.3433 (2)	0.3124 (1)	0.035 (1)
C(10*B*)	−0.4240 (3)	0.3491 (2)	0.3725 (1)	0.036 (1)
C(11′)	−0.5329 (3)	0.2211 (2)	0.1871 (1)	0.039 (1)
C(12′)	−0.5059 (3)	0.1996 (2)	0.1191 (1)	0.042 (1)
C(13′)	−0.5710 (5)	0.2521 (3)	0.0656 (2)	0.069 (2)
C(14′)	−0.5511 (6)	0.2309 (3)	0.0020 (2)	0.094 (2)
C(15′)	−0.4671 (6)	0.1558 (3)	−0.0082 (2)	0.088 (2)
C(16′)	−0.4043 (4)	0.1015 (3)	0.0446 (2)	0.077 (2)
C(17′)	−0.4236 (3)	0.1227 (3)	0.1081 (2)	0.055 (1)
C(18′)	−0.6291 (3)	0.1842 (2)	0.3309 (1)	0.037 (1)
C(19′)	−0.6382 (3)	0.0795 (2)	0.3406 (1)	0.035 (1)
C(20′)	−0.5371 (3)	0.0223 (2)	0.3149 (1)	0.039 (1)
C(21′)	−0.5555 (3)	−0.0741 (2)	0.3256 (2)	0.046 (1)
C(22′)	−0.6730 (3)	−0.1153 (2)	0.3639 (2)	0.050 (1)
C(23′)	−0.7738 (3)	−0.0601 (2)	0.3900 (2)	0.048 (1)
C(24′)	−0.7569 (3)	0.0372 (2)	0.3784 (1)	0.042 (1)
C(25′)	−0.4548 (3)	0.4129 (2)	0.2488 (2)	0.041 (1)
C(26′)	−0.5568 (3)	0.4479 (2)	0.1971 (2)	0.045 (1)
C(27′)	−0.5045 (4)	0.4909 (2)	0.1333 (2)	0.064 (1)
C(28′)	−0.5974 (6)	0.5269 (3)	0.0840 (2)	0.079 (2)
C(29′)	−0.7403 (6)	0.5199 (3)	0.0996 (2)	0.089 (2)
C(30′)	−0.7909 (5)	0.4779 (4)	0.1613 (2)	0.097 (2)
C(31′)	−0.7020 (4)	0.4415 (3)	0.2107 (2)	0.070 (2)

Table 2. *Selected geometric parameters (Å, °)*

O(2)—C(25)	1.217 (4)	O(1)—C(18)	1.213 (4)
C(10)—C(10*A*)	1.514 (4)	C(10)—C(9*A*)	1.577 (4)
C(10)—C(25)	1.527 (4)	C(10*A*)—C(1)	1.381 (5)
C(10*A*)—C(4*A*)	1.381 (4)	C(4*A*)—C(4*B*)	1.515 (4)
C(4*B*)—C(4*C*)	1.510 (4)	C(4*B*)—C(9*A*)	1.574 (4)
C(8*A*)—C(9)	1.479 (4)	C(4*C*)—C(8*A*)	1.387 (4)
C(9)—C(11)	1.332 (4)	C(9)—C(9*A*)	1.532 (4)
C(25)—C(26)	1.499 (4)	C(9*A*)—C(18)	1.537 (4)
C(11)—C(12)	1.470 (4)	C(18)—C(19)	1.498 (4)
C(10*A*)—C(10)—C(9*A*)	104.2 (2)	C(10*A*)—C(10)—C(25)	112.3 (2)
C(9*A*)—C(10)—C(25)	113.4 (2)	C(10)—C(10*A*)—C(1)	126.7 (2)
C(10)—C(10*A*)—C(4*A*)	112.1 (3)	C(10*A*)—C(4*A*)—C(4*B*)	111.4 (2)
C(4)—C(4*A*)—C(4*B*)	128.4 (3)	C(4*A*)—C(4*B*)—C(4*C*)	115.3 (2)
C(4*A*)—C(4*B*)—C(9*A*)	104.4 (2)	C(4*C*)—C(4*B*)—C(9*A*)	103.0 (2)
C(4*C*)—C(8*A*)—C(9)	110.7 (3)	C(4*B*)—C(4*C*)—C(8*A*)	111.9 (2)
C(8*A*)—C(9)—C(9*A*)	105.9 (2)	C(8)—C(8*A*)—C(9)	129.4 (3)
C(9*A*)—C(9)—C(11)	122.4 (3)	C(8*A*)—C(9)—C(11)	131.7 (3)
C(10)—C(9*A*)—C(9)	112.7 (2)	C(10)—C(9*A*)—C(4*B*)	105.3 (2)
C(10)—C(9*A*)—C(18)	109.9 (2)	C(4*B*)—C(9*A*)—C(9)	105.7 (2)
C(9)—C(9*A*)—C(18)	113.4 (2)	C(4*B*)—C(9*A*)—C(18)	109.4 (2)
O(2)—C(25)—C(26)	119.6 (3)	O(2)—C(25)—C(10)	120.5 (3)
C(25)—C(26)—C(27)	122.9 (3)	C(10)—C(25)—C(26)	119.9 (3)
O(1)—C(18)—C(9*A*)	120.0 (3)	O(1)—C(18)—C(19)	118.5 (2)
C(9*A*)—C(18)—C(19)	121.4 (2)	C(9)—C(11)—C(12)	129.2 (3)

The data reduction, structure solution and refinement were carried out using *SHELXTL-Plus* (VMS) (Sheldrick, 1991). The structure was solved by direct methods and refined successfully in the triclinic space group $P\bar{1}$, with two unique molecules per asymmetric unit. All non-H atoms were refined anisotropically to convergence, whereas H atoms were included in their calculated positions with fixed isotropic displacement parameters.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry, together with an ellipsoid plot of the second molecule in the asymmetric unit, have been deposited with the IUCr (Reference: AS1145). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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1-Iodo-2-methoxy-7-naphthyl Acetate

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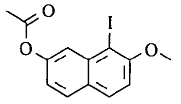
Abstract

The asymmetric unit of the title compound, $C_{13}H_{11}IO_3$, contains two independent molecules. The naphthalene ring systems of the molecules have average deviations from planarity of 0.029 (13) and 0.017 (9) Å with maximum deviations of 0.042 (11) and 0.034 (9) Å, respectively. The methyl parts of the methoxy groups are *anti*

to the neighboring α-C atoms and are nearly coplanar with the rings, with C—C—O—C torsion angles of −8.1 (15) and −3.7 (10)° in the two molecules. The dihedral angles between the naphthalene ring system and the acetate group in each molecule are 109.9 (2) and 114.6 (2)°.

Comment

The title compound, (I), was prepared by iodination of 2-acetoxy-7-methoxynaphthalene with elemental iodine (Sy, Lodge & By, 1990) in dichloromethane, as an intermediate in the synthesis of new binaphthylacetylenes (Prince, Evans, Rosas-García, Gandour & Fronczek, 1992).



(I)

The two molecules in the asymmetric unit, *A* and *B*, are related by an approximate inversion center. The midpoint between the two I atoms (0.4406, 0.5208, 0.6917) inverts one naphthalene ring system and methoxy group onto the other with deviations in the range 0.06–1.23 Å (average 0.61 Å). The acetoxy groups are less well related by inversion through this point.

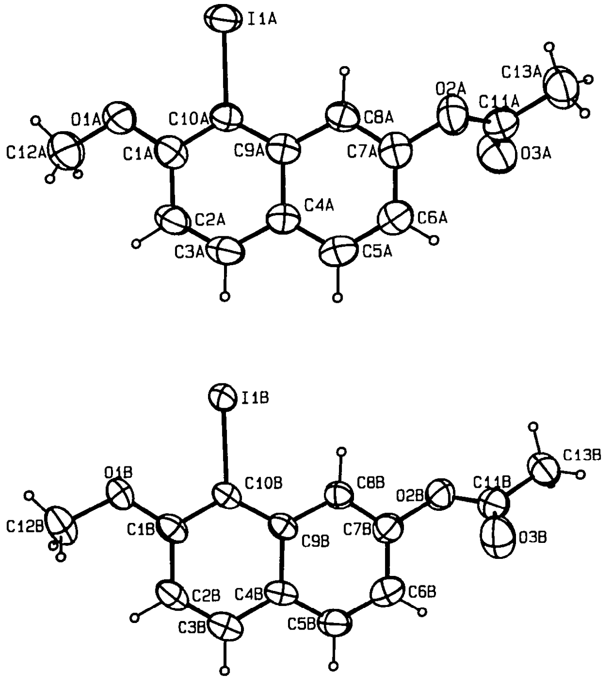


Fig. 1. Numbering scheme and displacement ellipsoids drawn at the 40% probability level for molecules *A* and *B*. H atoms are drawn as circles of arbitrary radii.

The methoxy O atom is closer to C10 than C2, as indicated by the difference in the angles O1—C1—C2 [124.3 (6) and 123.9 (6)°] and O1—C1—C10 [117.4 (6) and 116.9 (6)°]. This is explained by steric interaction between the methyl group and H2. This distortion is observed in similar 1-substituted 2-methoxynaphthalene structures (Prince, Fronczek & Gandour, 1989, 1990; Prince, Evans, Boss, Fronczek & Gandour, 1990). The methoxy group is twisted out of the naphthalene plane by slightly different amounts in the two independent molecules. The C2—C1—O1—C12 torsion angle is −8.1 (15)° in molecule *A* and −3.7 (10)° in molecule *B*. The carbonyl moiety lies out of the plane to avoid steric interaction with the H atoms on the ring. The conformation of the acetoxy group with respect to the aromatic ring also differs between the two molecules, with a C6—C7—O2—C11 torsion angle of 71.0 (11)° in molecule *A* and −66.2 (10)° in molecule *B*.

A search of the October 1992 version of the Cambridge Structural Database (Allen *et al.*, 1987) revealed no compound with an acetoxy substituent on position 2 or 7 of a naphthalene ring. Six 1-iodonaphthalene structures were found: see Cameron, Feutrill, Lammerts van Bueren, Raston & White (1977), and Cameron, Feutrill, Pannan, Raston, Skelton & White (1981). These have C—I distances in the range 2.01 (2)–2.11 (2) Å with an average of 2.085 (12) Å, which compares well with the average value of 2.087 (6) Å in (I).

Experimental

Colorless plates of (I), m.p. 376–378 K, were isolated by recrystallization from chloroform.

Crystal data

$C_{13}H_{11}IO_3$
$M_r = 342.1$
Monoclinic
$P2_1$
$a = 7.7051\ (9)$ Å
$b = 8.0610\ (8)$ Å
$c = 20.419\ (2)$ Å
$\beta = 93.338\ (9)°$
$V = 1266.1\ (4)$ Å^3
$Z = 4$
$D_x = 1.795$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–$13°$
$\mu = 2.5$ mm^{-1}
$T = 296$ K
Plate
0.62 × 0.52 × 0.05 mm
Colorless

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scans (North, Phillips & Mathews, 1968)
$T_{min} = 0.5670$, $T_{max} = 0.9998$
4173 measured reflections
3931 independent reflections

3382 observed reflections [$I > 3\sigma(I)$]
$R_{int} = 0.032$
$\theta_{max} = 30°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 11$
$l = -28 \rightarrow 28$
3 standard reflections
frequency: 166.67 min
intensity decay: <2%

Refinement

Refinement on F	$\Delta\rho_{max} = 1.10$ e Å^{-3}
$R = 0.0417$	$\Delta\rho_{min} = -0.23$ e Å^{-3}
$wR = 0.0485$	Extinction correction: none
$S = 2.493$	Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)
3382 reflections	
307 parameters	
H-atom parameters not refined	
$w = 4F_o^2/\sigma^2(F^2)$	
$(\Delta/\sigma)_{max} < 0.01$	

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
I1*A*	0.06011 (6)	0	0.57128 (2)	6.22 (1)
O1*A*	0.4315 (6)	0.123 (1)	0.6020 (3)	5.8 (1)
O2*A*	−0.1475 (6)	0.0129 (8)	0.3155 (2)	5.4 (1)
O3*A*	−0.0503 (7)	−0.2101 (9)	0.2655 (3)	6.8 (2)
C1*A*	0.4060 (9)	0.132 (1)	0.5356 (4)	4.7 (2)
C2*A*	0.5333 (9)	0.184 (1)	0.4932 (4)	5.5 (2)
C3*A*	0.499 (1)	0.193 (2)	0.4289 (4)	6.4 (2)
C4*A*	0.338 (1)	0.149 (1)	0.3984 (4)	4.9 (2)
C5*A*	0.299 (1)	0.166 (2)	0.3316 (4)	6.7 (2)
C6*A*	0.139 (1)	0.120 (1)	0.3034 (4)	5.7 (2)
C7*A*	0.0174 (8)	0.053 (1)	0.3436 (3)	4.6 (1)
C8*A*	0.0463 (7)	0.041 (1)	0.4086 (3)	4.2 (1)
C9*A*	0.2073 (8)	0.0888 (8)	0.4402 (3)	4.0 (1)
C10*A*	0.2443 (8)	0.0836 (9)	0.5081 (3)	3.9 (1)
C11*A*	−0.161 (1)	−0.117 (1)	0.2748 (4)	4.8 (2)
C12*A*	0.600 (1)	0.147 (2)	0.6317 (5)	7.5 (3)
C13*A*	−0.347 (1)	−0.125 (2)	0.2442 (5)	7.1 (3)
I1*B*	0.82111 (4)	1.0415 (1)	0.81204 (2)	3.880 (7)
O1*B*	0.4473 (5)	0.9365 (9)	0.7813 (2)	5.0 (1)
O2*B*	1.0728 (6)	0.8870 (8)	1.0565 (2)	4.8 (1)
O3*B*	0.9844 (7)	1.062 (1)	1.1336 (3)	6.9 (2)
C1*B*	0.4814 (7)	0.892 (1)	0.8449 (4)	3.9 (1)
C2*B*	0.3602 (8)	0.811 (1)	0.8835 (4)	4.7 (2)
C3*B*	0.4017 (9)	0.768 (1)	0.9468 (4)	4.9 (2)
C4*B*	0.5723 (8)	0.799 (1)	0.9753 (3)	4.0 (1)
C5*B*	0.6224 (9)	0.748 (1)	1.0394 (4)	4.9 (2)
C6*B*	0.785 (1)	0.778 (1)	1.0674 (4)	4.8 (2)
C7*B*	0.9012 (8)	0.862 (1)	1.0306 (3)	4.3 (1)
C8*B*	0.8638 (8)	0.914 (1)	0.9680 (3)	3.8 (1)
C9*B*	0.6967 (7)	0.8831 (8)	0.9382 (3)	3.4 (1)
C10*B*	0.6464 (7)	0.9271 (8)	0.8722 (3)	3.3 (1)
C11*B*	1.0983 (9)	0.987 (1)	1.1099 (3)	4.5 (1)
C12*B*	0.286 (1)	0.893 (1)	0.7494 (5)	5.7 (2)
C13*B*	1.2825 (9)	0.989 (1)	1.1338 (4)	5.3 (2)

Table 2. *Selected geometric parameters (Å, °)*

I1*A*—C10*A*	2.084 (6)	I1*B*—C10*B*	2.090 (6)
O1*A*—C1*A*	1.361 (9)	O1*B*—C1*B*	1.359 (9)
O1*A*—C12*A*	1.41 (1)	O1*B*—C12*B*	1.411 (9)
O2*A*—C7*A*	1.401 (8)	O2*B*—C7*B*	1.409 (8)
O2*A*—C11*A*	1.34 (1)	O2*B*—C11*B*	1.364 (9)
O3*A*—C11*A*	1.16 (1)	O3*B*—C11*B*	1.19 (1)
C1*A*—C2*A*	1.41 (1)	C1*B*—C2*B*	1.42 (1)
C1*A*—C10*A*	1.392 (9)	C1*B*—C10*B*	1.389 (8)
C2*A*—C3*A*	1.33 (1)	C2*B*—C3*B*	1.36 (1)
C3*A*—C4*A*	1.40 (1)	C3*B*—C4*B*	1.427 (9)
C4*A*—C5*A*	1.39 (1)	C4*B*—C5*B*	1.40 (1)
C4*A*—C9*A*	1.44 (1)	C4*B*—C9*B*	1.429 (9)
C5*A*—C6*A*	1.38 (1)	C5*B*—C6*B*	1.37 (1)
C6*A*—C7*A*	1.39 (1)	C6*B*—C7*B*	1.38 (1)
C7*A*—C8*A*	1.336 (9)	C7*B*—C8*B*	1.359 (9)
C8*A*—C9*A*	1.418 (9)	C8*B*—C9*B*	1.414 (8)
C9*A*—C10*A*	1.401 (9)	C9*B*—C10*B*	1.423 (9)
C11*A*—C13*A*	1.53 (1)	C11*B*—C13*B*	1.47 (1)
C1*A*—O1*A*—C12*A*	119.7 (6)	O2*A*—C11*A*—O3*A*	125.2 (7)
C7*A*—O2*A*—C11*A*	118.1 (6)	O2*A*—C11*A*—C13*A*	108.8 (7)
O1*A*—C1*A*—C2*A*	124.3 (6)	O3*A*—C11*A*—C13*A*	126.0 (8)
O1*A*—C1*A*—C10*A*	117.4 (6)	C1*B*—O1*B*—C12*B*	119.4 (6)
C2*A*—C1*A*—C10*A*	118.3 (7)	C7*B*—O2*B*—C11*B*	118.2 (5)
C1*A*—C2*A*—C3*A*	121.2 (7)	O1*B*—C1*B*—C2*B*	123.9 (6)
C2*A*—C3*A*—C4*A*	123.2 (8)	O1*B*—C1*B*—C10*B*	116.9 (6)
C3*A*—C4*A*—C5*A*	122.8 (9)	C2*B*—C1*B*—C10*B*	119.3 (6)
C3*A*—C4*A*—C9*A*	116.9 (7)	C1*B*—C2*B*—C3*B*	121.3 (6)
C5*A*—C4*A*—C9*A*	120.3 (7)	C2*B*—C3*B*—C4*B*	120.3 (7)
C4*A*—C5*A*—C6*A*	121.3 (8)	C3*B*—C4*B*—C5*B*	121.8 (7)
C5*A*—C6*A*—C7*A*	118.4 (7)	C3*B*—C4*B*—C9*B*	119.7 (6)
O2*A*—C7*A*—C6*A*	118.2 (6)	C5*B*—C4*B*—C9*B*	118.4 (6)
O2*A*—C7*A*—C8*A*	119.0 (6)	C4*B*—C5*B*—C6*B*	122.2 (7)
C6*A*—C7*A*—C8*A*	122.4 (7)	C5*B*—C6*B*—C7*B*	117.8 (7)
C7*A*—C8*A*—C9*A*	121.4 (6)	O2*B*—C7*B*—C6*B*	119.3 (6)
C4*A*—C9*A*—C8*A*	116.2 (6)	O2*B*—C7*B*—C8*B*	116.8 (6)
C4*A*—C9*A*—C10*A*	119.1 (6)	C6*B*—C7*B*—C8*B*	123.7 (6)
C8*A*—C9*A*—C10*A*	124.3 (6)	C7*B*—C8*B*—C9*B*	119.3 (6)
I1*A*—C10*A*—C1*A*	117.9 (5)	C4*B*—C9*B*—C8*B*	118.5 (6)
I1*A*—C10*A*—C9*A*	121.1 (4)	C4*B*—C9*B*—C10*B*	117.8 (5)
C1*A*—C10*A*—C9*A*	121.1 (6)	C8*B*—C9*B*—C10*B*	123.7 (6)
I1*B*—C10*B*—C1*B*	117.4 (5)	O2*B*—C11*B*—O3*B*	123.4 (6)
I1*B*—C10*B*—C9*B*	121.1 (4)	O2*B*—C11*B*—C13*B*	111.1 (6)
C1*B*—C10*B*—C9*B*	121.5 (6)	O3*B*—C11*B*—C13*B*	125.5 (7)

The I-atom positions were deduced from the Patterson function and the remainder of the non-H atoms were located using *DIRDIF* (Beurskens, 1984). H atoms were placed in calculated positions with C—H = 0.95 Å and $B_{iso} = 1.3B_{eq}$ of the C atoms to which they are bonded, using difference maps as a guide for methyl groups. In the weighting scheme, $\sigma^2(F^2) = S^2(C + R^2B) + (0.02F_o^2)^2/\text{Lp}^2$, where S = scan rate, C = total integrated peak count, R = ratio of scan to background counting times, B = total background count, and Lp = Lorentz–polarization factor. Refinement of the alternate absolute structure yielded $R = 0.0422$, $wR = 0.0492$, $S = 2.527$. Programs used include *MolEN* (Fair, 1990) and *ORTEP* (Johnson, 1965).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CR1135). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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trans-1,1′-Bis(indenylidene)

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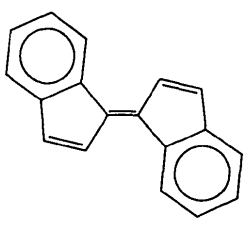
Abstract

The title compound, $(C_9H_6)_2$, was obtained by the coupling of the carbene C_9H_6: derived from 1-diazoindene, $C_9H_6N_2$, in the presence of $[Ru_3(CO)_{12}]$. The molecule is centrosymmetric and completely planar. The six-membered rings have aromatic character and are connected by an extended π-electron system.

Comment

In spite of being a relatively simple hydrocarbon, 1,1′-bis(indenylidene), (I), has not been described in the literature. It was obtained during our synthetic and structural studies on the reaction between metal carbonyl clusters and diazo compounds (Arce, De Sanctis, Manzur & Capparelli, 1994; Arce, De Sanctis, Machado, Manzur & Capparelli, 1995). The title compound was formed by the coupling of the carbene C_9H_6: derived from 1-diazoindene, $C_9H_6N_2$, in the presence of $[Ru_3(CO)_{12}]$.


(I)

The crystal structure analysis showed that the molecule of (I) (Fig. 1) is centrosymmetric and that the asymmetric unit consists of only one half of a molecule. The two halves are linked by a double bond, C1=C1^{i}, in a *trans* configuration imposed by the inversion centre. This bond and the double bond in the five-membered ring, C2=C3, form an hexatriene system (C3=C2—C1=C1^{i}—C2^{i}=C3^{i}). Within experimental error, both double bonds have equal lengths which are similar to the 1.345 (12) Å reported for hexatrienes (Allen *et al.*, 1987). The lengths of the single bonds (C1—C2, C1—C5 and C3—C4) indicate that they have partial double-bond character. The C1—C5 distance is comparable to 1.489 (5) Å, in agreement with equivalent bonds in five-membered rings (carbocyclic and heterocyclic) fused to benzene rings (Allen, 1981), but the C3—C4 bond length is significantly shorter. The C1—C2 distance is long when compared with 1.443 (13) Å for known hexatrienes (Allen *et al.*, 1987), or *ca* 1.44–1.47 Å observed in butadienes (Capparelli & Codding, 1993, and references therein). In general, the lengths of these $C_{sp^2}{=}C_{sp^2}$ double and $C_{sp^2}{-}C_{sp^2}$ single bonds reveal the existence of an extended π-electron system connecting both phenyl rings.

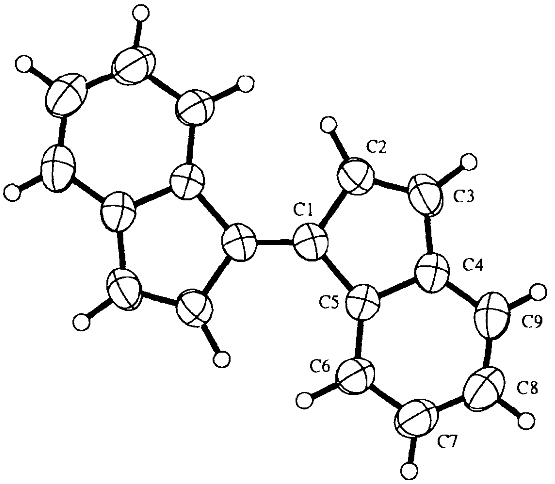


Fig. 1. Molecular structure of the title compound showing the displacement ellipsoids drawn at 40% probability.

The six-membered ring is aromatic and there is no indication that the ring fusion produces any double-bond fixation, in agreement with the findings of Allen (1981). In contrast, η^5 bonding of the five-membered rings to transition metals results in an aromatic character of these rings and a clear loss of aromaticity of the six-membered rings. This is indicated by the significant shortening of the C6—C7 and C8—C9 distances observed in $[Ru_3(C_{18}H_{12})(CO)_8]$, (II) (Arce, De Sanctis, Machado, Manzur & Capparelli, 1995). The average C—C bond length in the six-membered ring of (I), 1.386 (1) Å, coincides with the value given by Allen (1981) for benzene rings fused to five-membered rings. However,

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