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2,3-Diphenyl-1-indenone

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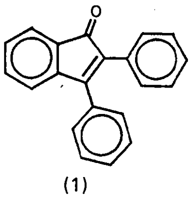
Abstract. $C_{21}H_{14}O$, $M_r = 282{\cdot}35$, monoclinic, $P2_1/n$, $a = 9{\cdot}503\ (1)$, $b = 17{\cdot}157\ (3)$, $c = 9{\cdot}894\ (1)$ Å, $\beta = 110{\cdot}723\ (9)°$, $V = 1508{\cdot}8\ (3)$ Å^3, $Z = 4$, $D_x = 1{\cdot}243$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}70$ cm^{-1}, $F(000) = 592$, $T = 293$ K, $R = 0{\cdot}0457$ for 1809 unique observed reflections. The indene moiety and attached atoms are planar (r.m.s.d. 0·03 Å), and the planar phenyl rings (0·006 and 0·007 Å r.m.s.d.'s) make angles of 52·6 (6) and 38·1 (6)° with the indene plane. The C(1)—C(2) double bond and attached atoms are statistically planar.

Experimental. Red, transparent crystal of (1) from benzene, 0·62 × 0·30 × 0·25 mm; Nicolet $R3m/\mu$ update of $P2_1$ diffractometer; data collected in Wyckoff mode (2θ fixed, ω varied, $3 \leq 2\theta \leq 50°$), variable scan rate (4 to 29·3° min^{-1}), graphite-monochromated Mo $K\alpha$ radiation; lattice parameters from a least-squares refinement of 25 reflections ($21{\cdot}77 \leq 2\theta \leq 35{\cdot}78°$), angles measured by a centering routine; systematic absences ($h0l$, $h+l = 2n+1$, $0k0$, $k = 2n+1$) consistent with space group $P2_1/n$, Laue symmetry $2/m$; monitored reflections $\bar{4}00$ and $\bar{1}\bar{9}1$ showed no statistically significant changes in intensities; 2656 independent reflections measured ($0 \leq h \leq 11$, $0 \leq k \leq 20$, $-11 \leq l \leq 10$), $1809 \geq 3{\cdot}0\sigma(I)$; Lorentz–polarization corrections, ψ-scan empirical absorption correction (transmission factors 0·899 to 0·980); structure solved by direct-methods techniques, block-cascade least-squares refinement with single isotropic temperature factor for all H atoms; $R = 0{\cdot}0457$, $wR = 0{\cdot}0359$ for 243 parameters and 1809 reflections ($R = 0{\cdot}0758$, $wR = 0{\cdot}0376$ for all 2656 reflections), $S = 1{\cdot}447$, $(\Delta/\sigma)_{\max} = 0{\cdot}019$, $(\Delta/\sigma)_{\text{av}} = 0{\cdot}006$; largest peaks in the final difference map of $+0{\cdot}15$ and $-0{\cdot}16$ e Å^{-3}, $\sum w(|F_o| - |F_c|)^2$ minimized with $w = [\sigma^2(F_o) + 0{\cdot}000039F_o^2]^{-1}$, extinction correc-



(1)

Table 1. *Atomic coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (Å^2 × 10^3)

	x	y	z	U_{eq}*
C(1)	6582 (2)	8667 (1)	1833 (2)	47 (1)
C(2)	7822 (2)	8813 (1)	1502 (2)	47 (1)
C(3)	7305 (2)	9049 (1)	−62 (2)	54 (1)
O	8102 (2)	9191 (1)	−759 (1)	72 (1)
C(4)	5639 (2)	9049 (1)	−587 (2)	53 (1)
C(5)	4605 (2)	9253 (1)	−1913 (2)	66 (1)
C(6)	3097 (3)	9223 (1)	−2078 (3)	74 (1)
C(7)	2652 (3)	8996 (1)	−959 (3)	70 (1)
C(8)	3709 (2)	8786 (1)	383 (2)	61 (1)
C(9)	5206 (2)	8812 (1)	554 (2)	50 (1)
C(11)	6512 (2)	8425 (1)	3243 (2)	51 (1)
C(12)	7329 (2)	8820 (1)	4499 (2)	62 (1)
C(13)	7292 (3)	8574 (2)	5818 (2)	78 (1)
C(14)	6447 (3)	7936 (2)	5886 (3)	86 (1)
C(15)	5626 (3)	7545 (1)	4655 (3)	80 (1)
C(16)	5641 (2)	7792 (1)	3327 (2)	63 (1)
C(21)	9420 (2)	8761 (1)	2410 (2)	49 (1)
C(22)	10434 (2)	9307 (1)	2262 (2)	59 (1)
C(23)	11933 (2)	9285 (1)	3132 (2)	68 (1)
C(24)	12448 (2)	8710 (2)	4158 (2)	72 (1)
C(25)	11460 (3)	8155 (1)	4300 (2)	70 (1)
C(26)	9969 (2)	8171 (1)	3438 (2)	57 (1)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

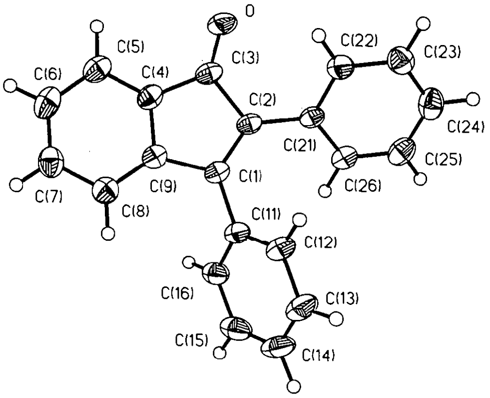


Fig. 1. Drawing of the title compound with thermal ellipsoids drawn at the 35% probability level and H atoms represented by spheres of arbitrary size.

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Table 2. *Bond lengths* (Å) *and valence angles* (°)

C(1)–C(2)	1·353 (3)	C(1)–C(9)	1·484 (2)
C(1)–C(11)	1·480 (3)	C(2)–C(3)	1·504 (2)
C(2)–C(21)	1·468 (2)	C(3)–O	1·216 (3)
C(3)–C(4)	1·482 (3)	C(4)–C(5)	1·377 (2)
C(4)–C(9)	1·391 (3)	C(5)–C(6)	1·385 (3)
C(6)–C(7)	1·374 (4)	C(7)–C(8)	1·399 (3)
C(8)–C(9)	1·373 (3)	C(11)–C(12)	1·387 (2)
C(11)–C(16)	1·386 (3)	C(12)–C(13)	1·384 (3)
C(13)–C(14)	1·373 (4)	C(14)–C(15)	1·367 (4)
C(15)–C(16)	1·386 (4)	C(21)–C(22)	1·389 (3)
C(21)–C(26)	1·398 (2)	C(22)–C(23)	1·379 (3)
C(23)–C(24)	1·376 (3)	C(24)–C(25)	1·379 (4)
C(25)–C(26)	1·371 (3)		

C(2)–C(1)–C(9)	110·0 (2)	C(2)–C(1)–C(11)	127·9 (1)
C(9)–C(1)–C(11)	122·1 (2)	C(1)–C(2)–C(3)	107·7 (1)
C(1)–C(2)–C(21)	129·9 (2)	C(3)–C(2)–C(21)	122·4 (2)
C(2)–C(3)–O	126·6 (2)	C(2)–C(3)–C(4)	106·2 (2)
O–C(3)–C(4)	127·2 (2)	C(3)–C(4)–C(5)	130·3 (2)
C(3)–C(4)–C(9)	107·6 (1)	C(5)–C(4)–C(9)	122·1 (2)
C(4)–C(5)–C(6)	117·5 (2)	C(5)–C(6)–C(7)	121·1 (2)
C(6)–C(7)–C(8)	121·0 (2)	C(7)–C(8)–C(9)	118·2 (2)
C(1)–C(9)–C(4)	108·4 (2)	C(1)–C(9)–C(8)	131·5 (2)
C(4)–C(9)–C(8)	120·0 (2)	C(1)–C(11)–C(12)	120·7 (2)
C(1)–C(11)–C(16)	120·2 (2)	C(12)–C(11)–C(16)	119·1 (2)
C(11)–C(12)–C(13)	120·2 (2)	C(12)–C(13)–C(14)	120·0 (2)
C(13)–C(14)–C(15)	120·4 (3)	C(14)–C(15)–C(16)	120·0 (2)
C(11)–C(16)–C(15)	120·2 (2)	C(2)–C(21)–C(22)	120·0 (2)
C(2)–C(21)–C(26)	121·9 (2)	C(22)–C(21)–C(26)	118·1 (2)
C(21)–C(22)–C(23)	121·2 (2)	C(22)–C(23)–C(24)	120·0 (2)
C(23)–C(24)–C(25)	119·5 (2)	C(24)–C(25)–C(26)	120·9 (2)
C(21)–C(26)–C(25)	120·3 (2)		

tion $F^* = F_c/[1{\cdot}0 + 0{\cdot}002gF_c^2/(\sin 2\theta)]^{0{\cdot}25}$ applied, g refined to 0·0033 (2). All computer programs supplied by Nicolet (Nicolet Instrument Corporation, 1986) for Desktop 30 Microeclipse and Nova 4/C configurations; atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). Table 1 lists atomic positional parameters, while Table 2 gives interatomic distances and valence angles.* The atom numbering is shown in Fig. 1.

Related literature. This study is part of an investigation of factors affecting the planarity of π-electron systems (Watson, 1983). The structure of dimethyl 3-phenylindene-1,2-dicarboxylate has been reported (Hanson, 1977).

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* Lists of H-atom coordinates, anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44245 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of (5*E*)-1α-Hydroxy-10β,14-epoxy-4(15),5-germacradiene-9-one*

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Abstract. $C_{15}H_{22}O_3$, $M_r = 250{\cdot}3$, monoclinic, $P2_1/c$, $a = 9{\cdot}936$ (2), $b = 5{\cdot}187$ (1), $c = 28{\cdot}852$ (5) Å, $\beta = 110{\cdot}77$ (1)°, $V = 1390{\cdot}3$ (4) Å^3, $Z = 4$, $D_m = 1{\cdot}20$ (1), $D_x = 1{\cdot}20$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}076$ mm^{-1}, $F(000) = 544{\cdot}2$, $T = 296$ (1) K, $R = 0{\cdot}049$ for 1586 unique observed reflections. To our disappointment, the relative configurations of this synthesized compound differ from those of (±)-periplanone B. However, the new synthetic compound will be used for biomimetic model reactions of a number of sesquiterpenes. The torsion angle of the C=C—C=C moiety is −53·2 (8)°. There is an intermolecular hydrogen bond, O—H···O, with O···O distance 2·836 (3) Å.

Experimental. The title compound was prepared from germacrene D isolated from the leaves of *Solidago*

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* This numbering is slightly different to that used within the paper.

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