

2-Methoxy-3,4-diphenylphenol

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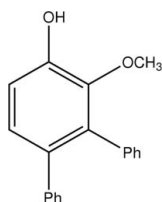
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Key indicators: single-crystal X-ray study; $T = 300$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.039; wR factor = 0.129; data-to-parameter ratio = 13.8.

The title compound, $\text{C}_{19}\text{H}_{16}\text{O}_2$, was isolated as the major product after the solid-state photochemical reaction of 2-methoxy-4,4-diphenylcyclohexa-2,5-dienone. The dihedral angles between the central ring and pendant benzene rings are 60.76 (6) and 51.64 (6)°. The O—C vector of the methoxy group is almost perpendicular to the plane of the central ring as indicated by the C—C—O—C torsion angle of 94.89 (18)°. Hydrogen-bonded dimers are formed in the crystal structure via O—H...O interactions. The data were collected at room temperature on a Bruker SMART X2S diffractometer in the automated mode and processed manually thereafter.

Related literature

For the characterization of reaction products, see: Frimer *et al.* (1994); Matoba *et al.* (1985). *Mogul* (Bruno *et al.*, 2002) was used for the geometrical analysis.



Experimental

Crystal data

$\text{C}_{19}\text{H}_{16}\text{O}_2$
 $M_r = 276.32$
 Monoclinic, $P2_1/c$

$a = 14.312$ (3) Å
 $b = 6.2585$ (14) Å
 $c = 17.167$ (4) Å

$\beta = 102.930$ (7)°
 $V = 1498.7$ (6) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.08$ mm⁻¹
 $T = 300$ K
 $0.36 \times 0.30 \times 0.28$ mm

Data collection

Bruker SMART X2S diffractometer
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2007)
 $T_{\min} = 0.972$, $T_{\max} = 0.978$

13658 measured reflections
 2645 independent reflections
 1897 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.129$
 $S = 1.01$
 2645 reflections

192 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.16$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³

Table 1
 Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H2}\cdots\text{O1}^i$	0.82	2.21	2.9043 (18)	142

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

Data collection: *GIS* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* and *OLEX2* (Dolomanov *et al.*, 2009); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: local programs (Guzei, 2007) and *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2575).

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supplementary materials

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2-Methoxy-3,4-diphenylphenol

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Comment

The title compound (I), Fig. 1, was isolated as the major product during our studies of the solid state photochemical behavior of 2-methoxy-4,4-diphenyl-2,5-cyclohexadienone as described in the Experimental.

All bond distances and angles in (I) fall in the expected ranges according to the *Mogul* structural check (Bruno, *et al.*, 2002). The dihedral angles between the C1—C6 ring and rings C8—C13 and C14—C19 are 60.76 (6)° and 51.64 (6)°, respectively. The O1—C7 vector of the methoxy group is almost perpendicular to the plane of the C1—C6 ring as indicated by the dihedral angle C2—C1—O1—C7 of 94.89 (18)°. Compound (I) forms hydrogen-bonded dimers in the solid state. The graph set notation for the dimers connected by O2—H2...O1 hydrogen bonds is R₂²(10).

Experimental

Solid state photolysis of 2-methoxy-4,4-diphenyl-2,5-cyclohexadienone (II) was studied as follows.

A thin film of (II) (0.30 g, 0.001 mol) was irradiated under nitrogen for 18 h through a CuSO₄ filter with a 400 watt medium pressure mercury lamp. The lamp was surrounded by a water-cooled immersion jacket and a cylindrical flask. The film of (II) was deposited on the inner wall of the outer flask (4 cm from the lamp) by slow evaporation of its dichloromethane solution and was dried before photolysis under nitrogen for 2 h. The resulting orange solid was chromatographed (silica gel 2.5 cm x 37 cm), eluted with hexane-CH₂Cl₂ (2:3) to give the following: band 1, 2-methoxy-4,5-diphenylphenol (III); band 2, 2-methoxy-3,4-diphenylphenol (I), band 3, 6-methoxy-5,6-diphenyl-2,4-cyclohexadienone (IV). The unreacted (band 4) cyclohexadienone (II) (0.10 g, 33%) was separated by using CH₂Cl₂—CH₃OH (9:1) elution (Scheme 1).

2-Methoxy-4,5-diphenylphenol (III) (Band 1): Recrystallization from ether-hexane gave (75 mg, 25%) colorless crystals, mp 419–421 K (Literature mp 422–423 K (Frimer *et al.*, 1994)). ¹H NMR (CDCl₃, 300 MHz): δ 3.95 (s, 3H), 5.62 (s, 1H), 6.91 (s, 1H), 7.02 (s, 1H), 7.10–7.21 (m, 10H) p.p.m.; ¹³C NMR (CDCl₃, 75 MHz) δ 56.3, 113.3, 116.9, 126.4, 128.0, 128.1, 130.2, 130.2, 133.3, 134.1, 141.6, 142.0, 145.1, 146.1 p.p.m.

2-Methoxy-3,4-diphenylphenol (I) (Band 2): Recrystallization from CH₂Cl₂-hexane gave (90 mg, 30%) colorless crystals, mp 417–419 K. ¹H NMR (CDCl₃, 300 MHz): δ 3.29 (s, 3H), 5.88 (s, 1H), 6.99–7.04 (m, 3H), 7.08–7.17 (m, 6H), 7.20–7.24 (m, 3H) p.p.m.; ¹³C NMR (CDCl₃, 75 MHz) δ 60.7, 114.5, 126.2, 126.8, 127.1, 127.8, 128.0, 130.2, 131.1, 133.8, 134.5, 136.3, 141.3, 145.3, 148.4 p.p.m.

6-Methoxy-5,6-diphenyl-2,4-cyclohexadienone (IV) (Band 3): This was recrystallized from CH₂Cl₂-hexane mixture. Yield = 15 mg, 5%; mp 467–469 K (Literature mp 469–471 K (Matoba *et al.*, 1985)). ¹H NMR (CDCl₃, 300 MHz): δ 3.66

supplementary materials

(s, 3H, OCH₃), 5.56 (d, *J* = 7.8 Hz, 1H), 5.88 (d, *J* = 9.9 Hz, 1H), 7.15–7.29 (m, 11H) p.p.m.; ¹³C NMR (CDCl₃, 75 MHz) δ 56.2, 69.5, 94.5, 118.8, 127.6, 128.3, 129.9, 141.0, 143.5, 171.2, 201.2 p.p.m.

Refinement

All H-atoms were placed in idealized locations (N—H = 0.82 Å and C—H = 0.93–0.96 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{bearing atom})$.

Figures

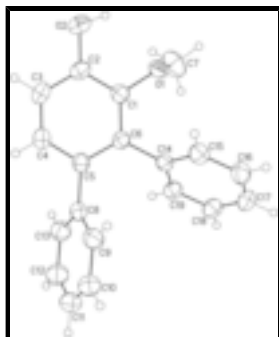


Fig. 1. Molecular structure of (I) showing the atom labelling and displacement ellipsoids at the 50% probability level.

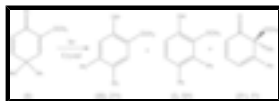


Fig. 2. The formation of the title compound.

2-Methoxy-3,4-diphenylphenol

Crystal data

C₁₉H₁₆O₂

$M_r = 276.32$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 14.312$ (3) Å

$b = 6.2585$ (14) Å

$c = 17.167$ (4) Å

$\beta = 102.930$ (7)°

$V = 1498.7$ (6) Å³

$Z = 4$

$F(000) = 584$

$D_x = 1.225$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 999 reflections

$\theta = 2.4\text{--}25.0^\circ$

$\mu = 0.08$ mm⁻¹

$T = 300$ K

Block, colourless

$0.36 \times 0.30 \times 0.28$ mm

Data collection

Bruker SMART X2S
diffractometer

Radiation source: micro-focus sealed tube
doubly curved silicon crystal

ω scans

2645 independent reflections

1897 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.4^\circ$

Absorption correction: multi-scan
(*SADABS*; Bruker, 2007) $h = -17 \rightarrow 17$
 $T_{\min} = 0.972$, $T_{\max} = 0.978$ $k = -7 \rightarrow 7$
 13658 measured reflections $l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.039$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.129$	H-atom parameters constrained
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.0877P)^2]$
2645 reflections	where $P = (F_o^2 + 2F_c^2)/3$
192 parameters	$(\Delta/\sigma)_{\max} < 0.001$
0 restraints	$\Delta\rho_{\max} = 0.16 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.40221 (7)	0.44465 (18)	0.45356 (6)	0.0466 (3)
O2	0.55156 (8)	0.1831 (2)	0.44401 (8)	0.0630 (4)
H2	0.5431	0.2608	0.4803	0.095*
C1	0.39866 (10)	0.3357 (2)	0.38259 (9)	0.0388 (4)
C2	0.47494 (10)	0.2000 (3)	0.38019 (10)	0.0443 (4)
C3	0.47283 (12)	0.0780 (3)	0.31276 (11)	0.0501 (5)
H3	0.5228	-0.0155	0.3110	0.060*
C4	0.39596 (11)	0.0956 (3)	0.24786 (10)	0.0453 (4)
H4	0.3945	0.0107	0.2031	0.054*
C5	0.32054 (10)	0.2373 (2)	0.24768 (9)	0.0388 (4)
C6	0.32128 (10)	0.3600 (2)	0.31656 (9)	0.0352 (4)
C7	0.35107 (16)	0.3378 (4)	0.50515 (13)	0.0751 (6)
H7A	0.2843	0.3301	0.4795	0.113*
H7C	0.3586	0.4158	0.5543	0.113*

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H7B	0.3761	0.1960	0.5162	0.113*
C8	0.24411 (10)	0.2612 (3)	0.17289 (10)	0.0413 (4)
C9	0.22906 (13)	0.4551 (3)	0.13291 (11)	0.0532 (5)
H9	0.2650	0.5736	0.1542	0.064*
C10	0.16117 (15)	0.4750 (4)	0.06154 (12)	0.0648 (6)
H10	0.1522	0.6063	0.0355	0.078*
C11	0.10739 (14)	0.3023 (4)	0.02930 (12)	0.0668 (6)
H11	0.0620	0.3157	-0.0185	0.080*
C12	0.12096 (13)	0.1098 (4)	0.06801 (13)	0.0660 (6)
H12	0.0843	-0.0074	0.0463	0.079*
C13	0.18878 (12)	0.0874 (3)	0.13916 (11)	0.0532 (5)
H13	0.1974	-0.0447	0.1646	0.064*
C14	0.24119 (10)	0.5068 (2)	0.32365 (9)	0.0368 (4)
C15	0.25989 (12)	0.7172 (3)	0.34987 (10)	0.0464 (4)
H15	0.3223	0.7691	0.3600	0.056*
C16	0.18630 (14)	0.8488 (3)	0.36086 (11)	0.0580 (5)
H16	0.1996	0.9883	0.3785	0.070*
C17	0.09338 (14)	0.7743 (3)	0.34579 (12)	0.0634 (5)
H17	0.0441	0.8626	0.3538	0.076*
C18	0.07375 (12)	0.5682 (3)	0.31880 (12)	0.0577 (5)
H18	0.0110	0.5179	0.3081	0.069*
C19	0.14693 (11)	0.4360 (3)	0.30755 (10)	0.0456 (4)
H19	0.1328	0.2975	0.2889	0.055*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0403 (6)	0.0606 (8)	0.0379 (6)	-0.0037 (5)	0.0068 (5)	-0.0070 (5)
O2	0.0436 (7)	0.0751 (10)	0.0632 (9)	0.0138 (6)	-0.0030 (6)	-0.0042 (7)
C1	0.0354 (8)	0.0435 (9)	0.0389 (9)	-0.0043 (6)	0.0114 (7)	-0.0017 (7)
C2	0.0323 (8)	0.0502 (10)	0.0499 (10)	0.0019 (7)	0.0081 (7)	0.0050 (8)
C3	0.0415 (9)	0.0498 (11)	0.0617 (12)	0.0109 (7)	0.0172 (8)	0.0012 (8)
C4	0.0473 (9)	0.0456 (10)	0.0466 (10)	0.0035 (7)	0.0184 (8)	-0.0033 (8)
C5	0.0401 (8)	0.0402 (9)	0.0387 (9)	-0.0003 (6)	0.0141 (7)	0.0010 (7)
C6	0.0315 (7)	0.0378 (8)	0.0377 (9)	-0.0010 (6)	0.0106 (6)	0.0030 (7)
C7	0.0934 (15)	0.0886 (16)	0.0522 (12)	-0.0144 (12)	0.0352 (11)	-0.0028 (11)
C8	0.0425 (8)	0.0460 (10)	0.0377 (9)	0.0045 (7)	0.0138 (7)	-0.0020 (7)
C9	0.0626 (11)	0.0505 (11)	0.0455 (10)	0.0042 (8)	0.0099 (8)	0.0000 (8)
C10	0.0763 (14)	0.0673 (13)	0.0487 (12)	0.0224 (11)	0.0096 (10)	0.0073 (10)
C11	0.0560 (11)	0.0907 (16)	0.0481 (12)	0.0149 (11)	-0.0003 (9)	-0.0069 (11)
C12	0.0487 (10)	0.0768 (15)	0.0670 (14)	-0.0026 (9)	0.0013 (9)	-0.0157 (11)
C13	0.0493 (10)	0.0531 (11)	0.0555 (11)	-0.0016 (8)	0.0082 (8)	-0.0036 (9)
C14	0.0367 (8)	0.0420 (9)	0.0320 (8)	0.0018 (6)	0.0081 (6)	-0.0003 (7)
C15	0.0510 (9)	0.0437 (10)	0.0446 (10)	-0.0018 (7)	0.0111 (7)	0.0000 (8)
C16	0.0765 (13)	0.0435 (11)	0.0527 (11)	0.0110 (9)	0.0116 (10)	-0.0052 (9)
C17	0.0588 (11)	0.0742 (14)	0.0566 (12)	0.0296 (10)	0.0112 (9)	-0.0059 (10)
C18	0.0369 (9)	0.0767 (14)	0.0582 (12)	0.0099 (8)	0.0075 (8)	-0.0063 (10)
C19	0.0365 (8)	0.0506 (10)	0.0489 (10)	0.0018 (7)	0.0075 (7)	-0.0051 (8)

Geometric parameters (Å, °)

O1—C1	1.3871 (18)	C9—H9	0.9300
O1—C7	1.434 (2)	C10—C11	1.370 (3)
O2—C2	1.3698 (19)	C10—H10	0.9300
O2—H2	0.8200	C11—C12	1.368 (3)
C1—C2	1.391 (2)	C11—H11	0.9300
C1—C6	1.405 (2)	C12—C13	1.387 (3)
C2—C3	1.382 (2)	C12—H12	0.9300
C3—C4	1.384 (2)	C13—H13	0.9300
C3—H3	0.9300	C14—C19	1.388 (2)
C4—C5	1.397 (2)	C14—C15	1.398 (2)
C4—H4	0.9300	C15—C16	1.383 (2)
C5—C6	1.408 (2)	C15—H15	0.9300
C5—C8	1.496 (2)	C16—C17	1.378 (3)
C6—C14	1.495 (2)	C16—H16	0.9300
C7—H7A	0.9600	C17—C18	1.378 (3)
C7—H7C	0.9600	C17—H17	0.9300
C7—H7B	0.9600	C18—C19	1.382 (2)
C8—C9	1.387 (2)	C18—H18	0.9300
C8—C13	1.393 (2)	C19—H19	0.9300
C9—C10	1.389 (3)		
C1—O1—C7	112.95 (13)	C10—C9—H9	119.5
C2—O2—H2	109.5	C11—C10—C9	120.29 (19)
O1—C1—C2	116.83 (13)	C11—C10—H10	119.9
O1—C1—C6	121.54 (13)	C9—C10—H10	119.9
C2—C1—C6	121.63 (14)	C12—C11—C10	119.52 (18)
O2—C2—C3	119.41 (14)	C12—C11—H11	120.2
O2—C2—C1	121.10 (15)	C10—C11—H11	120.2
C3—C2—C1	119.49 (15)	C11—C12—C13	120.80 (19)
C2—C3—C4	119.66 (15)	C11—C12—H12	119.6
C2—C3—H3	120.2	C13—C12—H12	119.6
C4—C3—H3	120.2	C12—C13—C8	120.53 (17)
C3—C4—C5	121.82 (16)	C12—C13—H13	119.7
C3—C4—H4	119.1	C8—C13—H13	119.7
C5—C4—H4	119.1	C19—C14—C15	118.20 (14)
C4—C5—C6	118.94 (14)	C19—C14—C6	121.10 (14)
C4—C5—C8	118.79 (14)	C15—C14—C6	120.66 (13)
C6—C5—C8	122.20 (13)	C16—C15—C14	120.53 (16)
C1—C6—C5	118.38 (13)	C16—C15—H15	119.7
C1—C6—C14	118.76 (13)	C14—C15—H15	119.7
C5—C6—C14	122.79 (13)	C17—C16—C15	120.36 (17)
O1—C7—H7A	109.5	C17—C16—H16	119.8
O1—C7—H7C	109.5	C15—C16—H16	119.8
H7A—C7—H7C	109.5	C18—C17—C16	119.70 (16)
O1—C7—H7B	109.5	C18—C17—H17	120.2
H7A—C7—H7B	109.5	C16—C17—H17	120.2
H7C—C7—H7B	109.5	C17—C18—C19	120.23 (17)

supplementary materials

C9—C8—C13	117.81 (16)	C17—C18—H18	119.9
C9—C8—C5	120.99 (15)	C19—C18—H18	119.9
C13—C8—C5	121.14 (15)	C18—C19—C14	120.97 (16)
C8—C9—C10	121.06 (18)	C18—C19—H19	119.5
C8—C9—H9	119.5	C14—C19—H19	119.5
C7—O1—C1—C2	-94.89 (18)	C6—C5—C8—C13	-123.15 (17)
C7—O1—C1—C6	84.55 (18)	C13—C8—C9—C10	-0.1 (3)
O1—C1—C2—O2	-2.8 (2)	C5—C8—C9—C10	177.00 (16)
C6—C1—C2—O2	177.77 (14)	C8—C9—C10—C11	0.1 (3)
O1—C1—C2—C3	176.31 (14)	C9—C10—C11—C12	0.1 (3)
C6—C1—C2—C3	-3.1 (2)	C10—C11—C12—C13	-0.3 (3)
O2—C2—C3—C4	-179.50 (15)	C11—C12—C13—C8	0.4 (3)
C1—C2—C3—C4	1.4 (2)	C9—C8—C13—C12	-0.2 (2)
C2—C3—C4—C5	1.3 (3)	C5—C8—C13—C12	-177.25 (16)
C3—C4—C5—C6	-2.3 (2)	C1—C6—C14—C19	-125.28 (16)
C3—C4—C5—C8	174.84 (15)	C5—C6—C14—C19	51.8 (2)
O1—C1—C6—C5	-177.28 (13)	C1—C6—C14—C15	52.1 (2)
C2—C1—C6—C5	2.1 (2)	C5—C6—C14—C15	-130.82 (16)
O1—C1—C6—C14	-0.1 (2)	C19—C14—C15—C16	1.3 (2)
C2—C1—C6—C14	179.32 (14)	C6—C14—C15—C16	-176.18 (15)
C4—C5—C6—C1	0.6 (2)	C14—C15—C16—C17	-0.2 (3)
C8—C5—C6—C1	-176.46 (13)	C15—C16—C17—C18	-0.7 (3)
C4—C5—C6—C14	-176.52 (13)	C16—C17—C18—C19	0.6 (3)
C8—C5—C6—C14	6.5 (2)	C17—C18—C19—C14	0.5 (3)
C4—C5—C8—C9	-117.18 (18)	C15—C14—C19—C18	-1.4 (2)
C6—C5—C8—C9	59.8 (2)	C6—C14—C19—C18	176.05 (15)
C4—C5—C8—C13	59.8 (2)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2 \cdots O1 ⁱ	0.82	2.21	2.9043 (18)	142

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

Fig. 1

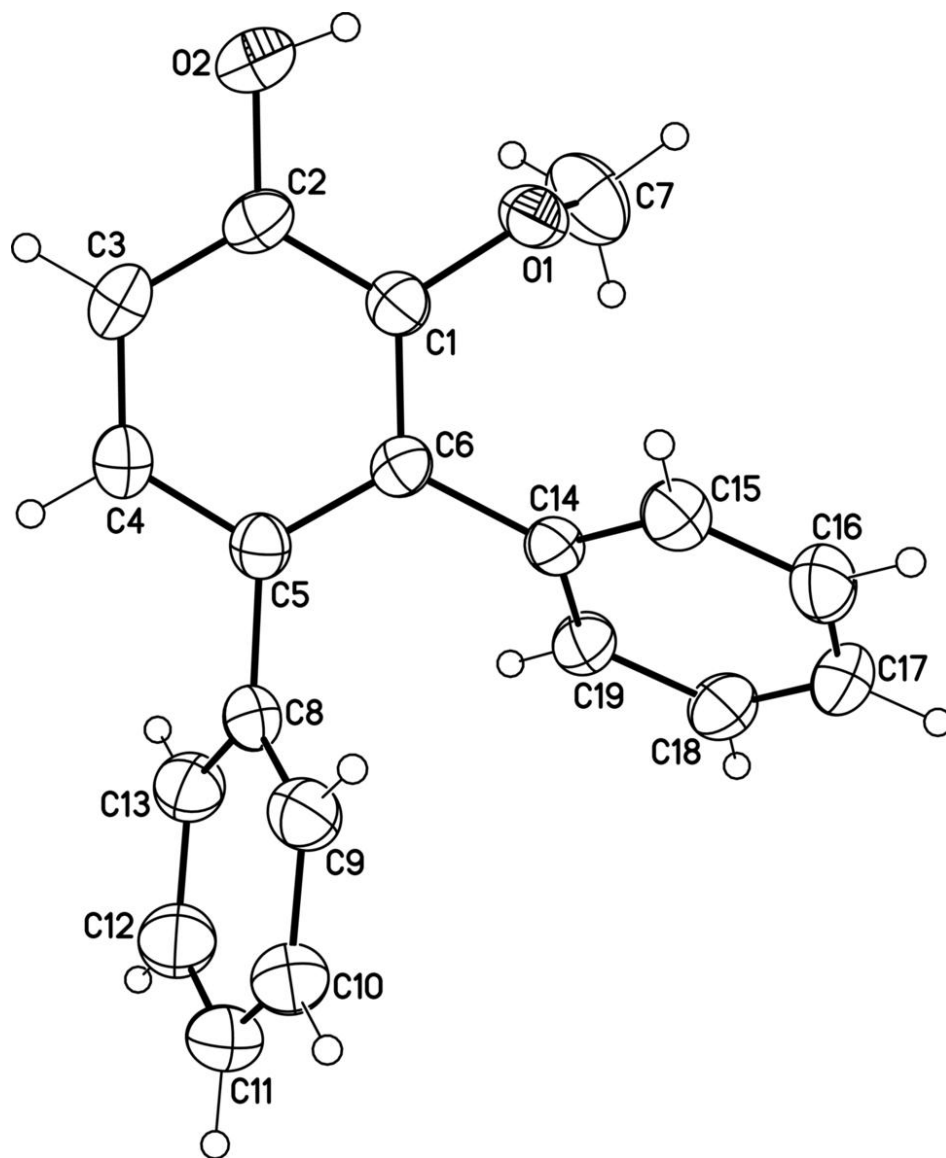


Fig. 2

