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2,6-Bis(3,4-dimethoxybenzylidene)-4-ethylcyclohexanone

Rajeev Mudakavi,[a] Brinda,[a] M. Srinivas Murthy,[b] Deepak Chopra[a]* and T. N. Guru Row[a]

[a]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, India, and [b]Department of Pharmaceutical Chemistry, Al-Ameen College of Pharmacy, Bangalore 560 027, Karnataka, India
Correspondence e-mail: deepak@sscu.iisc.ernet.in

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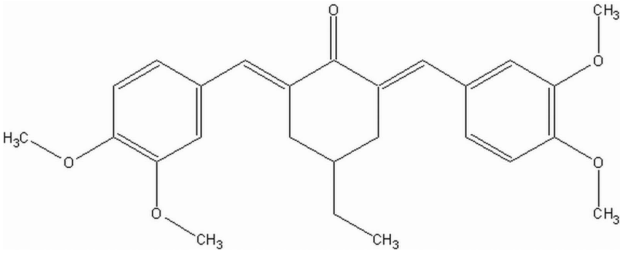
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; R factor = 0.069; wR factor = 0.182; data-to-parameter ratio = 18.5.

In the title compound, $C_{26}H_{30}O_5$, both the double bonds exist in an E configuration. The aryl rings are not coplanar with the adjacent olefinic groups owing to non-bonded interactions between the *ortho* H atoms of the aryl rings and the equatorial H atoms at the 3- and 5-positions of the cyclohexyl ring; the dihedral angles between the aryl rings and the olefinic groups are 33.7 (3) and 48.6 (4)°. The cyclohexanone ring adopts an envelope conformation and the crystal structure is stabilized by C—H···O hydrogen bonds.

Related literature

For related structures, see: Dimmock *et al.* (2001, 2005). For related literature, see: Bernstein *et al.* (1995); Cremer & Pople (1975).



Experimental

Crystal data

$C_{26}H_{30}O_5$
M_r = 422.5
Monoclinic, $P2_1/n$
a = 10.3766 (10) Å
b = 8.6973 (9) Å
c = 24.555 (3) Å
β = 93.500 (2)°
V = 2212.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 273 (2) K
0.25 × 0.21 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.983, T_{max} = 0.986
18534 measured reflections
5285 independent reflections
3034 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.182
S = 1.02
5285 reflections
285 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14B···O2^{i}	0.96	2.54	3.410 (3)	151

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{5}{2}$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

We thank the Department of Science and Technology, India, for data collection on the CCD facility set up under the IRHPA–DST program. DC thanks the Indian Institute of Science for a fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2382).

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supplementary materials

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2,6-Bis(3,4-dimethoxybenzylidene)-4-ethylcyclohexanone

R. Mudakavi, Brinda, M. S. Murthy, D. Chopra and T. N. G. Row

Comment

Substituted 2,6-bis(benzylidenecyclohexanone) derivatives have been the subject of recent crystallographic investigations and have found useful applications as potent anti-cancer agents (Dimmock *et al.*, 2001, 2005).

The six-membered cyclohexanone ring exists in an envelope conformation, the Cremer and Pople puckering parameters are Q(T) = 0.546 (2) Å, φ(2) = 172.5 (3)°, θ (2) = 57.3 (2)° (Cremer and Pople, 1975). The ring atom C24 deviates by +0.406 (6)Å from the least squares plane passing through C2/C4/C7/C8/C17. The C24 ring atom deviates by +0.406 (6)Å from the least squares plane passing through C2/C4/C7/C8/C17. Also the C6—C7—C8, 129.8 (2) and C2—C16—C17 130.2 (2) ° angles and the torsion angles about the C7—C8 24.4 (4) ° and C16—C17 − 31.9 (4)° bonds also deviate from planarity indicating significant steric repulsion between the aryl ring and the cyclohexanone ring, with repulsions in particular between the hydrogen atoms H18···H3B, 2.284 Å and H9···H5A 2.209 Å respectively. The crystal packing is stabilized by C—H···O intermolecular interactions forming C(7) molecular chains (Bernstein *et al.*, 1995) along the crystallographic *b* axis.

Experimental

An aqueous solution of sodium hydroxide (10% *w*/*v*, 30 ml) was added to a solution of 3,4-dimethoxybenzaldehyde (3.32 g, 0.02 mol) and γ-ethylcyclohexanone (1.4 ml, 0.01 mol) in ethanol (50 ml). The reaction mixture was stirred at 10–20 ° for 2 hr and left overnight in an ice chest forming a yellow colored solid. The product was filtered, washed with ice-cold water (100 ml) followed by ice-cold ethanol (20 ml), dried and recrystallized from alcohol. The yield of product, m.p.138–139 °, was 81%.

Refinement

All the H atoms were located in a difference Fourier map and refined isotropically with C—H bond lengths in the range 0.89 (4)–0.94 (3) Å.

Figures

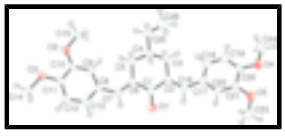

Fig. 1. Molecular structure of (I), showing 50% ellipsoidal probability.

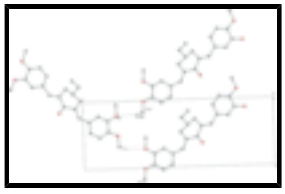

Fig. 2. Packing diagram of (I). The dotted lines show C—H···O hydrogen bonds.

2,6-Bis(3,4-dimethoxybenzylidene)-4-ethylcyclohexanone

Crystal data

$C_{26}H_{30}O_5$	F_{000} = 904
M_r = 422.5	D_x = 1.269 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 670.44 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 10.3766 (10) Å	Cell parameters from 2836 reflections
b = 8.6973 (9) Å	θ = 2.5–23.5º
c = 24.555 (3) Å	μ = 0.09 mm^{-1}
β = 93.500 (2)º	T = 273 (2) K
V = 2212.0 (4) Å^3	Block, yellow
Z = 4	0.25 × 0.21 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer	5285 independent reflections
Radiation source: fine-focus sealed tube	3034 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 273(2) K	θ_{max} = 28.3º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1997)	h = −13→11
T_{min} = 0.983, T_{max} = 0.986	k = −11→11
18534 measured reflections	l = −31→32

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.069	H-atom parameters constrained
$wR(F^2)$ = 0.182	$w = 1/[\sigma^2(F_o^2) + (0.0842P)^2 + 0.3153P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
5285 reflections	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
285 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.25921 (17)	−0.51272 (18)	1.18110 (6)	0.0502 (5)
O4	0.08370 (19)	0.64202 (18)	0.69106 (7)	0.0559 (5)
O2	0.25180 (18)	−0.21513 (17)	1.17688 (6)	0.0508 (5)
C10	0.2184 (2)	−0.2892 (2)	1.12918 (8)	0.0371 (5)
C11	0.2215 (2)	−0.4510 (2)	1.13192 (8)	0.0373 (5)
O1	0.0307 (2)	−0.1498 (2)	0.87689 (8)	0.0793 (7)
O5	0.0943 (2)	0.36852 (19)	0.64952 (7)	0.0633 (6)
C8	0.1502 (2)	−0.3001 (3)	1.03314 (9)	0.0384 (6)
C21	0.0922 (3)	0.3754 (3)	0.70512 (9)	0.0445 (6)
C2	0.1249 (2)	0.0979 (3)	0.88009 (9)	0.0392 (6)
C9	0.1824 (2)	−0.2170 (3)	1.08089 (9)	0.0388 (6)
H9	0.1793	−0.1102	1.0799	0.047*
C6	0.1473 (2)	−0.0922 (3)	0.96042 (9)	0.0405 (6)
C16	0.0823 (2)	0.1245 (3)	0.82837 (9)	0.0435 (6)
H16	0.0433	0.0407	0.8105	0.052*
C7	0.1164 (2)	−0.2306 (3)	0.97992 (9)	0.0425 (6)
H7	0.0658	−0.2916	0.9560	0.051*
C17	0.0875 (2)	0.2643 (3)	0.79554 (9)	0.0410 (6)
C15	0.2665 (3)	−0.0521 (3)	1.17406 (10)	0.0536 (7)
H15A	0.3298	−0.0273	1.1485	0.080*
H15B	0.2942	−0.0131	1.2094	0.080*
H15C	0.1854	−0.0061	1.1623	0.080*
C22	0.0908 (2)	0.2500 (3)	0.73870 (9)	0.0450 (6)
H22	0.0921	0.1522	0.7234	0.054*
C12	0.1847 (3)	−0.5342 (3)	1.08564 (9)	0.0454 (6)
H12	0.1831	−0.6411	1.0871	0.054*
C3	0.2037 (2)	0.2092 (3)	0.91474 (9)	0.0446 (6)
H3A	0.1474	0.2671	0.9373	0.053*
H3B	0.2458	0.2813	0.8914	0.053*
C20	0.0866 (2)	0.5240 (3)	0.72757 (9)	0.0428 (6)
C13	0.1501 (2)	−0.4595 (3)	1.03715 (9)	0.0451 (6)

H13	0.1261	−0.5176	1.0064	0.054*
C4	0.3058 (2)	0.1258 (3)	0.95126 (9)	0.0439 (6)
H4	0.3560	0.0601	0.9280	0.053*
C1	0.0966 (3)	−0.0552 (3)	0.90345 (9)	0.0467 (6)
C18	0.0819 (2)	0.4114 (3)	0.81681 (9)	0.0468 (6)
H18	0.0779	0.4244	0.8543	0.056*
C19	0.0819 (2)	0.5396 (3)	0.78330 (10)	0.0458 (6)
H19	0.0788	0.6373	0.7986	0.055*
C25	0.3987 (3)	0.2322 (3)	0.98288 (10)	0.0538 (7)
H25A	0.3496	0.3000	1.0052	0.065*
H25B	0.4549	0.1709	1.0073	0.065*
C5	0.2348 (2)	0.0220 (3)	0.98994 (9)	0.0469 (6)
H5A	0.2978	−0.0330	1.0133	0.056*
H5B	0.1840	0.0856	1.0130	0.056*
C23	0.1095 (3)	0.2212 (3)	0.62546 (10)	0.0645 (8)
H23A	0.1869	0.1738	0.6409	0.097*
H23B	0.1153	0.2325	0.5868	0.097*
H23C	0.0365	0.1579	0.6324	0.097*
C14	0.2557 (3)	−0.6761 (3)	1.18519 (10)	0.0549 (7)
H14A	0.1693	−0.7117	1.1766	0.082*
H14B	0.2829	−0.7065	1.2217	0.082*
H14C	0.3126	−0.7201	1.1600	0.082*
C24	0.0659 (3)	0.7937 (3)	0.71203 (12)	0.0623 (8)
H24A	−0.0154	0.7991	0.7286	0.093*
H24B	0.0667	0.8668	0.6827	0.093*
H24C	0.1345	0.8170	0.7388	0.093*
C26	0.4803 (3)	0.3281 (4)	0.94805 (13)	0.0776 (10)
H26A	0.5198	0.2635	0.9221	0.116*
H26B	0.5462	0.3786	0.9706	0.116*
H26C	0.4274	0.4038	0.9290	0.116*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0763 (13)	0.0321 (9)	0.0405 (9)	−0.0047 (8)	−0.0098 (8)	0.0072 (7)
O4	0.0767 (14)	0.0348 (10)	0.0564 (11)	0.0028 (9)	0.0048 (9)	0.0091 (8)
O2	0.0826 (14)	0.0329 (9)	0.0354 (8)	−0.0086 (9)	−0.0088 (8)	−0.0009 (7)
C10	0.0446 (15)	0.0325 (12)	0.0340 (11)	−0.0060 (11)	0.0015 (10)	−0.0025 (9)
C11	0.0442 (15)	0.0307 (12)	0.0370 (11)	−0.0031 (11)	0.0022 (10)	0.0050 (9)
O1	0.1210 (19)	0.0558 (12)	0.0556 (11)	−0.0415 (12)	−0.0395 (12)	0.0182 (9)
O5	0.1096 (17)	0.0416 (10)	0.0383 (9)	0.0034 (10)	0.0019 (10)	0.0059 (8)
C8	0.0440 (15)	0.0341 (13)	0.0367 (11)	−0.0055 (11)	−0.0010 (10)	0.0011 (9)
C21	0.0544 (16)	0.0406 (14)	0.0381 (12)	0.0009 (12)	−0.0001 (11)	0.0034 (10)
C2	0.0421 (15)	0.0370 (13)	0.0379 (12)	−0.0053 (11)	−0.0024 (10)	0.0036 (10)
C9	0.0467 (15)	0.0297 (12)	0.0399 (12)	−0.0039 (11)	0.0016 (10)	0.0019 (9)
C6	0.0458 (15)	0.0403 (13)	0.0347 (11)	−0.0070 (11)	−0.0035 (10)	0.0044 (10)
C16	0.0499 (16)	0.0379 (13)	0.0422 (12)	−0.0054 (12)	−0.0020 (11)	0.0003 (10)
C7	0.0522 (16)	0.0406 (14)	0.0337 (11)	−0.0078 (12)	−0.0050 (10)	0.0017 (10)

C17	0.0415 (15)	0.0405 (13)	0.0402 (12)	−0.0008 (11)	−0.0037 (10)	0.0040 (10)
C15	0.078 (2)	0.0309 (13)	0.0502 (14)	−0.0101 (13)	−0.0094 (13)	−0.0047 (11)
C22	0.0561 (17)	0.0352 (13)	0.0427 (13)	−0.0005 (12)	−0.0051 (11)	0.0019 (10)
C12	0.0659 (18)	0.0269 (12)	0.0429 (13)	−0.0043 (12)	0.0008 (12)	0.0004 (10)
C3	0.0537 (17)	0.0400 (14)	0.0392 (12)	−0.0122 (12)	−0.0044 (11)	0.0056 (10)
C20	0.0465 (16)	0.0339 (13)	0.0474 (13)	−0.0002 (11)	−0.0026 (11)	0.0078 (10)
C13	0.0622 (18)	0.0353 (13)	0.0370 (12)	−0.0063 (12)	−0.0046 (11)	−0.0066 (10)
C4	0.0526 (16)	0.0398 (13)	0.0385 (12)	−0.0080 (12)	−0.0035 (11)	−0.0001 (10)
C1	0.0550 (17)	0.0428 (14)	0.0408 (13)	−0.0099 (12)	−0.0100 (11)	0.0046 (11)
C18	0.0528 (17)	0.0500 (15)	0.0370 (12)	0.0004 (13)	−0.0019 (11)	0.0000 (11)
C19	0.0480 (16)	0.0385 (14)	0.0505 (14)	0.0006 (12)	−0.0007 (11)	−0.0041 (11)
C25	0.0548 (18)	0.0519 (16)	0.0538 (15)	−0.0122 (13)	−0.0032 (13)	−0.0014 (12)
C5	0.0546 (17)	0.0461 (14)	0.0384 (12)	−0.0137 (12)	−0.0099 (11)	0.0069 (11)
C23	0.098 (3)	0.0528 (17)	0.0424 (14)	0.0097 (16)	0.0054 (15)	−0.0049 (12)
C14	0.081 (2)	0.0314 (13)	0.0509 (15)	0.0020 (13)	−0.0035 (14)	0.0093 (11)
C24	0.079 (2)	0.0330 (14)	0.0750 (19)	0.0041 (14)	0.0029 (16)	0.0057 (13)
C26	0.069 (2)	0.087 (2)	0.077 (2)	−0.0365 (19)	0.0017 (17)	−0.0004 (18)

Geometric parameters (Å, °)

O3—C11	1.357 (2)	C22—H22	0.9300
O3—C14	1.425 (3)	C12—C13	1.384 (3)
O4—C20	1.362 (3)	C12—H12	0.9300
O4—C24	1.432 (3)	C3—C4	1.528 (3)
O2—C10	1.363 (2)	C3—H3A	0.9700
O2—C15	1.429 (3)	C3—H3B	0.9700
C10—C9	1.373 (3)	C20—C19	1.379 (3)
C10—C11	1.409 (3)	C13—H13	0.9300
C11—C12	1.382 (3)	C4—C25	1.516 (3)
O1—C1	1.231 (3)	C4—C5	1.532 (3)
O5—C21	1.368 (3)	C4—H4	0.9800
O5—C23	1.424 (3)	C18—C19	1.386 (3)
C8—C13	1.390 (3)	C18—H18	0.9300
C8—C9	1.400 (3)	C19—H19	0.9300
C8—C7	1.463 (3)	C25—C26	1.494 (4)
C21—C22	1.368 (3)	C25—H25A	0.9700
C21—C20	1.407 (3)	C25—H25B	0.9700
C2—C16	1.339 (3)	C5—H5A	0.9700
C2—C1	1.486 (3)	C5—H5B	0.9700
C2—C3	1.499 (3)	C23—H23A	0.9600
C9—H9	0.9300	C23—H23B	0.9600
C6—C7	1.341 (3)	C23—H23C	0.9600
C6—C1	1.499 (3)	C14—H14A	0.9600
C6—C5	1.502 (3)	C14—H14B	0.9600
C16—C17	1.462 (3)	C14—H14C	0.9600
C16—H16	0.9300	C24—H24A	0.9600
C7—H7	0.9300	C24—H24B	0.9600
C17—C18	1.384 (3)	C24—H24C	0.9600
C17—C22	1.404 (3)	C26—H26A	0.9600

C15—H15A	0.9600	C26—H26B	0.9600
C15—H15B	0.9600	C26—H26C	0.9600
C15—H15C	0.9600		
C11—O3—C14	116.73 (18)	C12—C13—C8	121.9 (2)
C20—O4—C24	117.13 (19)	C12—C13—H13	119.1
C10—O2—C15	116.75 (17)	C8—C13—H13	119.1
O2—C10—C9	124.6 (2)	C25—C4—C3	114.0 (2)
O2—C10—C11	115.29 (19)	C25—C4—C5	110.94 (19)
C9—C10—C11	120.1 (2)	C3—C4—C5	107.5 (2)
O3—C11—C12	125.1 (2)	C25—C4—H4	108.1
O3—C11—C10	116.22 (19)	C3—C4—H4	108.1
C12—C11—C10	118.7 (2)	C5—C4—H4	108.1
C21—O5—C23	117.55 (18)	O1—C1—C2	120.7 (2)
C13—C8—C9	117.2 (2)	O1—C1—C6	120.2 (2)
C13—C8—C7	118.3 (2)	C2—C1—C6	119.1 (2)
C9—C8—C7	124.5 (2)	C17—C18—C19	121.2 (2)
O5—C21—C22	124.6 (2)	C17—C18—H18	119.4
O5—C21—C20	115.8 (2)	C19—C18—H18	119.4
C22—C21—C20	119.6 (2)	C20—C19—C18	120.7 (2)
C16—C2—C1	117.3 (2)	C20—C19—H19	119.6
C16—C2—C3	124.3 (2)	C18—C19—H19	119.6
C1—C2—C3	118.26 (19)	C26—C25—C4	114.4 (2)
C10—C9—C8	121.7 (2)	C26—C25—H25A	108.7
C10—C9—H9	119.1	C4—C25—H25A	108.7
C8—C9—H9	119.1	C26—C25—H25B	108.7
C7—C6—C1	116.6 (2)	C4—C25—H25B	108.7
C7—C6—C5	124.9 (2)	H25A—C25—H25B	107.6
C1—C6—C5	118.41 (19)	C6—C5—C4	112.95 (18)
C2—C16—C17	130.2 (2)	C6—C5—H5A	109.0
C2—C16—H16	114.9	C4—C5—H5A	109.0
C17—C16—H16	114.9	C6—C5—H5B	109.0
C6—C7—C8	129.8 (2)	C4—C5—H5B	109.0
C6—C7—H7	115.1	H5A—C5—H5B	107.8
C8—C7—H7	115.1	O5—C23—H23A	109.5
C18—C17—C22	117.5 (2)	O5—C23—H23B	109.5
C18—C17—C16	123.8 (2)	H23A—C23—H23B	109.5
C22—C17—C16	118.6 (2)	O5—C23—H23C	109.5
O2—C15—H15A	109.5	H23A—C23—H23C	109.5
O2—C15—H15B	109.5	H23B—C23—H23C	109.5
H15A—C15—H15B	109.5	O3—C14—H14A	109.5
O2—C15—H15C	109.5	O3—C14—H14B	109.5
H15A—C15—H15C	109.5	H14A—C14—H14B	109.5
H15B—C15—H15C	109.5	O3—C14—H14C	109.5
C21—C22—C17	122.0 (2)	H14A—C14—H14C	109.5
C21—C22—H22	119.0	H14B—C14—H14C	109.5
C17—C22—H22	119.0	O4—C24—H24A	109.5
C11—C12—C13	120.4 (2)	O4—C24—H24B	109.5
C11—C12—H12	119.8	H24A—C24—H24B	109.5
C13—C12—H12	119.8	O4—C24—H24C	109.5

C2—C3—C4	111.17 (19)	H24A—C24—H24C	109.5
C2—C3—H3A	109.4	H24B—C24—H24C	109.5
C4—C3—H3A	109.4	C25—C26—H26A	109.5
C2—C3—H3B	109.4	C25—C26—H26B	109.5
C4—C3—H3B	109.4	H26A—C26—H26B	109.5
H3A—C3—H3B	108.0	C25—C26—H26C	109.5
O4—C20—C19	125.3 (2)	H26A—C26—H26C	109.5
O4—C20—C21	115.7 (2)	H26B—C26—H26C	109.5
C19—C20—C21	119.0 (2)		
C15—O2—C10—C9	−8.7 (3)	C24—O4—C20—C19	−4.3 (4)
C15—O2—C10—C11	171.9 (2)	C24—O4—C20—C21	174.4 (2)
C14—O3—C11—C12	−2.3 (3)	O5—C21—C20—O4	0.1 (3)
C14—O3—C11—C10	176.6 (2)	C22—C21—C20—O4	−177.7 (2)
O2—C10—C11—O3	−1.1 (3)	O5—C21—C20—C19	178.9 (2)
C9—C10—C11—O3	179.5 (2)	C22—C21—C20—C19	1.0 (4)
O2—C10—C11—C12	177.8 (2)	C11—C12—C13—C8	−0.4 (4)
C9—C10—C11—C12	−1.6 (4)	C9—C8—C13—C12	−2.3 (4)
C23—O5—C21—C22	−6.8 (4)	C7—C8—C13—C12	178.1 (2)
C23—O5—C21—C20	175.5 (2)	C2—C3—C4—C25	173.6 (2)
O2—C10—C9—C8	179.5 (2)	C2—C3—C4—C5	−63.0 (2)
C11—C10—C9—C8	−1.2 (4)	C16—C2—C1—O1	−3.8 (4)
C13—C8—C9—C10	3.1 (4)	C3—C2—C1—O1	178.9 (3)
C7—C8—C9—C10	−177.3 (2)	C16—C2—C1—C6	177.4 (2)
C1—C2—C16—C17	175.7 (3)	C3—C2—C1—C6	0.2 (3)
C3—C2—C16—C17	−7.2 (4)	C7—C6—C1—O1	−0.3 (4)
C1—C6—C7—C8	−180.0 (2)	C5—C6—C1—O1	175.9 (3)
C5—C6—C7—C8	4.1 (4)	C7—C6—C1—C2	178.5 (2)
C13—C8—C7—C6	−156.0 (3)	C5—C6—C1—C2	−5.3 (4)
C9—C8—C7—C6	24.4 (4)	C22—C17—C18—C19	−1.2 (4)
C2—C16—C17—C18	−31.9 (4)	C16—C17—C18—C19	−177.3 (2)
C2—C16—C17—C22	152.0 (3)	O4—C20—C19—C18	178.2 (2)
O5—C21—C22—C17	−179.4 (2)	C21—C20—C19—C18	−0.4 (4)
C20—C21—C22—C17	−1.8 (4)	C17—C18—C19—C20	0.5 (4)
C18—C17—C22—C21	1.9 (4)	C3—C4—C25—C26	−63.4 (3)
C16—C17—C22—C21	178.2 (2)	C5—C4—C25—C26	175.0 (3)
O3—C11—C12—C13	−178.8 (2)	C7—C6—C5—C4	151.2 (3)
C10—C11—C12—C13	2.4 (4)	C1—C6—C5—C4	−24.7 (3)
C16—C2—C3—C4	−142.5 (3)	C25—C4—C5—C6	−176.5 (2)
C1—C2—C3—C4	34.5 (3)	C3—C4—C5—C6	58.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14B···O2^{i}	0.96	2.54	3.410 (3)	151

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+5/2.

Fig. 1

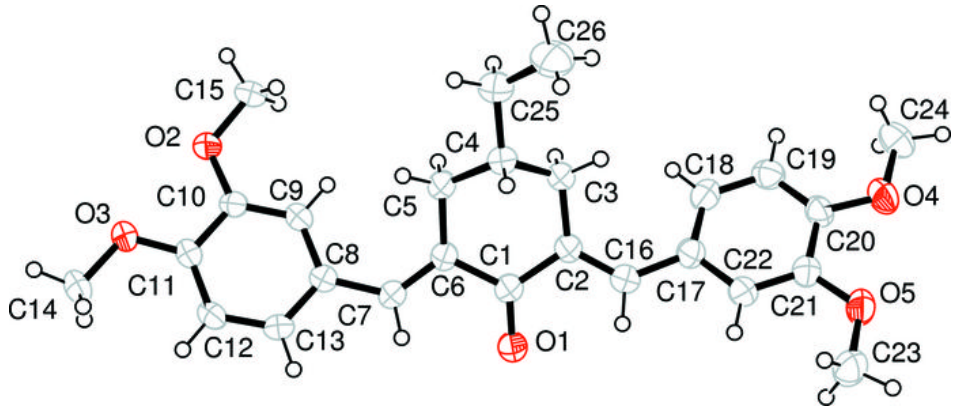
C26
C25
C15
O2
C4
C24
C18
C19
C10
C9
C5
C3
O4
O3
C8
C1
C16
C22
C20
C11
C6
C2
C17
C21
O5
C14
C7
C12
C13
O1
C23

Fig. 2