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2,6-Di-*tert*-butyl-4-(methoxymethyl)-phenol

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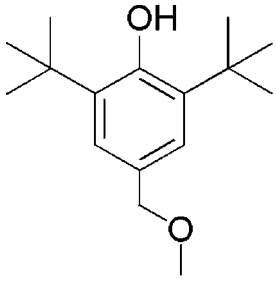
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.060; wR factor = 0.190; data-to-parameter ratio = 14.4.

The title compound, $C_{16}H_{26}O_2$, was easily obtained in high yield when 4-bromomethyl-2,6-di-*tert*-butylphenol was reacted with methanol. There are two independent molecules in the asymmetric unit. The methoxy group in each of the independent molecules was found to be disordered, with site-occupation factors of 0.8728 (18)/0.1272 (18) and 0.8781 (17)/0.1219 (17).

Related literature

For related literature, see: Rieker *et al.* (1968); Yamazaki & Seguchi (1997); Zeng *et al.* (2005).



Experimental

Crystal data

$C_{16}H_{26}O_2$
M_r = 250.37
Monoclinic, $P2_1/c$
a = 14.240 (3) Å
b = 18.012 (3) Å
c = 13.677 (3) Å
β = 118.603 (3)°
V = 3079.7 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 294 (2) K
0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.982, T_{max} = 0.986
15799 measured reflections
5428 independent reflections
2928 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.189
S = 1.04
5428 reflections
378 parameters
108 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ER2048).

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Rieker, A., Kaufmann, D., Brück, R., Workman, R. & Müller, E. (1968). *Tetrahedron*, **24**, 103–115.
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Yamazaki, T. & Seguchi, T. (1997). *J. Polym. Sci. A: Polym. Chem.* **35**, 2431–2439.
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supplementary materials

Acta Cryst. (2008). E**64**, o588 [**doi:10.1107/S1600536808003644**]

2,6-Di-*tert*-butyl-4-(methoxymethyl)phenol

T. Zeng and J.-F. Sun

Comment

Hindered phenol antioxidants are widely used in polymers and lubricants. It could protect polymers by increasing both their process stability and long-term stability against oxidative degradation (Yamazaki & Seguchi, 1997). In former papers, we have reported the reaction of 4-bromomethyl-20,6-di-tet-butyl-phenol with amines (Zeng *et al.*, 2005) and it was showed that the 4-bromomethyl-2,6-di-tet-butyl-phenol was highly reactive. The title compound, $C_{16}H_{26}O_2$,(1),has been easily synthesied when we tried to dissolve the 4-bromomethyl-2,6-di-*tert*-butyl-phenol in methanol. It was found that there are two independent molecules in the asymmetric units. The phenolic hydroxyl are hindered by the adjacent *tert*-butyl groups. And both of the methoxyl groups in the two molecules were found disordered with with site occupation fators 0.8728 (18)/ 0.1272 (18) and 0.8781 (17)/0.1219 (17).

Experimental

The 4-bromomethyl-2,6-di-*tert*-butyl-phenol (7.15 g) was synthesized from 2,6-di-*tert*-butyl-4-methylphenol (5.5 g, 0.025 mol) and equivalent NBS (Rieker *et al.*, 1968) in a yield of 96%. Then 40 ml me thanol was added and stirred for 5 min the produt (5.85 g, 0.023 mol) was obtained in a yield of 97.3%. Suitable crystals were obtained by slow evaporation of a mixture of ethyl acetate and ethanol.

Refinement

The H atoms of O—H were initially located in a difference Fourier Map and restrained on their parent atoms with O—H restrained 0.82 Å. In absence of significant anomalous dispersion effects, Friedel-pair reflections were merged prior to refinement. All H other atoms were positioned geometrically and refined using a riding model, in the range of 0.93–0.97 Å, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C_{methyl})$.

Figures

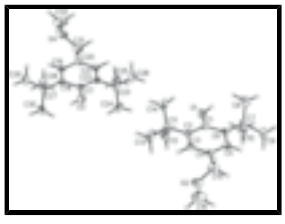


Fig. 1. The two independent molecules in the structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

2,6-di-*tert*-butyl-4-(methoxymethyl)phenol

Crystal data

$C_{16}H_{26}O_2$	F_{000} = 1104
M_r = 250.37	D_x = 1.080 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 14.240 (3) Å	Cell parameters from 2933 reflections
b = 18.012 (3) Å	θ = 2.8–25.4º
c = 13.677 (3) Å	μ = 0.07 mm^{-1}
β = 118.603 (3)º	T = 294 (2) K
V = 3079.7 (10) Å^3	Block, colourless
Z = 8	0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer	5428 independent reflections
Radiation source: fine-focus sealed tube	2928 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	h = −13→16
T_{min} = 0.982, T_{max} = 0.986	k = −20→21
15799 measured reflections	l = −16→10

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.060	H-atom parameters constrained
$wR(F^2)$ = 0.189	$w = 1/[\sigma^2(F_o^2) + (0.0751P)^2 + 1.0963P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.002
5428 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
378 parameters	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
108 restraints	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0102 (7)

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
O1	0.29438 (11)	0.73376 (8)	0.66027 (11)	0.0698 (5)	
H1	0.2550	0.7700	0.6367	0.105*	
O3	0.20663 (10)	0.25936 (8)	0.37111 (12)	0.0701 (4)	
H3	0.2381	0.2196	0.3821	0.105*	
C1	0.35866 (12)	0.74063 (10)	0.77320 (14)	0.0425 (5)	
C2	0.39601 (12)	0.67334 (9)	0.83200 (14)	0.0410 (5)	
C3	0.46179 (12)	0.67844 (10)	0.94611 (14)	0.0448 (5)	
H3A	0.4869	0.6349	0.9871	0.054*	
C4	0.49145 (12)	0.74549 (10)	1.00116 (14)	0.0453 (5)	
C5	0.45463 (13)	0.80952 (10)	0.94014 (15)	0.0501 (5)	
H5	0.4756	0.8548	0.9771	0.060*	
C6	0.38758 (12)	0.80988 (10)	0.82580 (15)	0.0450 (5)	
C7	0.34673 (15)	0.88356 (11)	0.76197 (18)	0.0626 (6)	
C8	0.22446 (17)	0.88849 (13)	0.7136 (2)	0.0880 (9)	
H8A	0.1995	0.9353	0.6763	0.132*	
H8B	0.2067	0.8845	0.7728	0.132*	
H8C	0.1910	0.8488	0.6614	0.132*	
C9	0.3953 (2)	0.95088 (12)	0.8398 (2)	0.0973 (10)	
H9A	0.4714	0.9513	0.8684	0.146*	
H9B	0.3796	0.9474	0.9006	0.146*	
H9C	0.3651	0.9958	0.7990	0.146*	
C10	0.37776 (19)	0.89054 (13)	0.6695 (2)	0.0911 (8)	
H10A	0.3479	0.9354	0.6282	0.137*	
H10B	0.3506	0.8486	0.6205	0.137*	
H10C	0.4543	0.8920	0.7020	0.137*	
C11	0.36507 (14)	0.59799 (10)	0.77160 (16)	0.0528 (6)	
C12	0.40573 (18)	0.59247 (12)	0.68675 (19)	0.0808 (8)	
H12A	0.3708	0.6292	0.6298	0.121*	
H12B	0.3904	0.5439	0.6537	0.121*	
H12C	0.4816	0.6008	0.7234	0.121*	
C13	0.41538 (18)	0.53359 (11)	0.8551 (2)	0.0815 (9)	
H13A	0.3971	0.4872	0.8157	0.122*	
H13B	0.3886	0.5343	0.9076	0.122*	

H13C	0.4917	0.5392	0.8940	0.122*	
C14	0.24411 (16)	0.58545 (12)	0.7145 (2)	0.0785 (8)	
H14A	0.2089	0.6230	0.6588	0.118*	
H14B	0.2197	0.5881	0.7688	0.118*	
H14C	0.2277	0.5374	0.6800	0.118*	
C17	0.14067 (12)	0.25795 (10)	0.41872 (14)	0.0428 (5)	
C18	0.11153 (12)	0.19114 (9)	0.44964 (14)	0.0424 (5)	
C19	0.04478 (13)	0.19708 (10)	0.49784 (14)	0.0473 (5)	
H19	0.0243	0.1539	0.5200	0.057*	
C20	0.00815 (12)	0.26412 (10)	0.51383 (14)	0.0463 (5)	
C21	0.03681 (13)	0.32793 (10)	0.47987 (14)	0.0469 (5)	
H21	0.0107	0.3731	0.4894	0.056*	
C22	0.10338 (13)	0.32747 (10)	0.43179 (14)	0.0435 (5)	
C23	0.13593 (15)	0.40024 (10)	0.39658 (16)	0.0565 (6)	
C24	0.25658 (16)	0.41172 (13)	0.4620 (2)	0.0821 (8)	
H24A	0.2748	0.4583	0.4412	0.123*	
H24B	0.2920	0.3721	0.4456	0.123*	
H24C	0.2789	0.4120	0.5402	0.123*	
C25	0.0990 (2)	0.39898 (13)	0.27121 (18)	0.0843 (8)	
H25A	0.1168	0.4453	0.2495	0.126*	
H25B	0.0230	0.3916	0.2308	0.126*	
H25C	0.1342	0.3592	0.2549	0.126*	
C26	0.08391 (18)	0.46798 (11)	0.4192 (2)	0.0839 (8)	
H26A	0.1046	0.4700	0.4971	0.126*	
H26B	0.0075	0.4639	0.3766	0.126*	
H26C	0.1071	0.5124	0.3982	0.126*	
C27	0.15203 (15)	0.11556 (11)	0.43482 (17)	0.0591 (6)	
C28	0.12020 (19)	0.10122 (12)	0.3133 (2)	0.0873 (8)	
H28A	0.0437	0.1021	0.2696	0.131*	
H28B	0.1465	0.0535	0.3064	0.131*	
H28C	0.1503	0.1390	0.2872	0.131*	
C29	0.10241 (17)	0.05158 (11)	0.4707 (2)	0.0827 (8)	
H29A	0.1247	0.0559	0.5487	0.124*	
H29B	0.1260	0.0048	0.4566	0.124*	
H29C	0.0258	0.0544	0.4290	0.124*	
C30	0.27315 (16)	0.11003 (13)	0.5082 (2)	0.0907 (9)	
H30A	0.3074	0.1487	0.4885	0.136*	
H30B	0.2974	0.0626	0.4973	0.136*	
H30C	0.2907	0.1153	0.5849	0.136*	
C15	0.55793 (15)	0.75095 (12)	1.12630 (15)	0.0648 (6)	0.8728 (18)
H15A	0.5955	0.7980	1.1459	0.078*	0.8728 (18)
H15B	0.5114	0.7492	1.1598	0.078*	0.8728 (18)
O2	0.63105 (11)	0.69353 (9)	1.16775 (11)	0.0614 (5)	0.8728 (18)
C16	0.6887 (2)	0.69504 (18)	1.28628 (18)	0.0875 (10)	0.8728 (18)
H16A	0.7390	0.6548	1.3127	0.131*	0.8728 (18)
H16B	0.6397	0.6901	1.3155	0.131*	0.8728 (18)
H16C	0.7264	0.7413	1.3106	0.131*	0.8728 (18)
C15'	0.5580 (8)	0.7510 (7)	1.1264 (5)	0.0648 (6)	0.1272 (18)
H15C	0.5102	0.7640	1.1557	0.078*	0.1272 (18)

H15D	0.5856	0.7018	1.1541	0.078*	0.1272 (18)
O2'	0.6430 (6)	0.7997 (6)	1.1711 (6)	0.105 (6)	0.1272 (18)
C16'	0.6844 (13)	0.7853 (10)	1.2889 (7)	0.073 (5)	0.1272 (18)
H16D	0.7463	0.8156	1.3310	0.110*	0.1272 (18)
H16E	0.7037	0.7339	1.3040	0.110*	0.1272 (18)
H16F	0.6306	0.7969	1.3097	0.110*	0.1272 (18)
C31	−0.0573 (9)	0.2684 (4)	0.5737 (4)	0.0646 (6)	0.8781 (17)
H31A	−0.0098	0.2663	0.6533	0.078*	0.8781 (17)
H31B	−0.0948	0.3154	0.5568	0.078*	0.8781 (17)
O4	−0.13064 (10)	0.21107 (9)	0.54314 (11)	0.0608 (5)	0.8781 (17)
C32	−0.18536 (18)	0.21175 (19)	0.6076 (2)	0.0943 (11)	0.8781 (17)
H32A	−0.2358	0.1716	0.5845	0.141*	0.8781 (17)
H32B	−0.2226	0.2580	0.5966	0.141*	0.8781 (17)
H32C	−0.1345	0.2061	0.6850	0.141*	0.8781 (17)
C31'	−0.0573 (9)	0.2684 (4)	0.5737 (4)	0.0646 (6)	0.1219 (17)
H31C	−0.0839	0.2190	0.5752	0.078*	0.1219 (17)
H31D	−0.0106	0.2831	0.6501	0.078*	0.1219 (17)
O4'	−0.1426 (5)	0.3164 (5)	0.5280 (6)	0.071 (3)	0.1219 (17)
C32'	−0.1973 (8)	0.3038 (9)	0.5923 (9)	0.060 (4)	0.1219 (17)
H32D	−0.2571	0.3371	0.5676	0.089*	0.1219 (17)
H32E	−0.1489	0.3125	0.6697	0.089*	0.1219 (17)
H32F	−0.2224	0.2535	0.5823	0.089*	0.1219 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0750 (9)	0.0690 (9)	0.0423 (8)	0.0148 (7)	0.0095 (7)	0.0070 (7)
O3	0.0796 (7)	0.0652 (9)	0.0971 (8)	0.0051 (7)	0.0677 (6)	0.0076 (7)
C1	0.0349 (8)	0.0530 (10)	0.0384 (9)	0.0040 (8)	0.0167 (7)	0.0026 (8)
C2	0.0342 (8)	0.0445 (10)	0.0426 (9)	0.0019 (7)	0.0171 (7)	0.0041 (8)
C3	0.0345 (8)	0.0532 (10)	0.0451 (9)	0.0028 (8)	0.0178 (7)	0.0099 (8)
C4	0.0330 (8)	0.0600 (11)	0.0424 (9)	−0.0013 (8)	0.0177 (7)	−0.0034 (9)
C5	0.0427 (8)	0.0513 (11)	0.0595 (10)	−0.0009 (8)	0.0272 (8)	−0.0114 (9)
C6	0.0379 (8)	0.0463 (10)	0.0548 (10)	0.0044 (8)	0.0255 (7)	0.0010 (8)
C7	0.0625 (11)	0.0460 (11)	0.0771 (13)	0.0114 (9)	0.0318 (10)	0.0058 (10)
C8	0.0754 (13)	0.0737 (15)	0.1056 (18)	0.0319 (12)	0.0358 (13)	0.0151 (13)
C9	0.1047 (17)	0.0478 (13)	0.126 (2)	0.0059 (13)	0.0441 (15)	−0.0020 (14)
C10	0.1118 (16)	0.0688 (14)	0.1058 (16)	0.0121 (13)	0.0626 (13)	0.0317 (13)
C11	0.0470 (9)	0.0475 (11)	0.0550 (11)	−0.0020 (8)	0.0172 (8)	0.0005 (9)
C12	0.0961 (14)	0.0655 (14)	0.0892 (15)	−0.0035 (12)	0.0511 (12)	−0.0236 (12)
C13	0.0829 (15)	0.0466 (12)	0.0873 (17)	−0.0029 (11)	0.0184 (13)	0.0079 (12)
C14	0.0588 (12)	0.0702 (14)	0.0853 (16)	−0.0185 (11)	0.0174 (12)	−0.0097 (12)
C17	0.0356 (7)	0.0538 (11)	0.0412 (9)	−0.0024 (8)	0.0201 (7)	0.0017 (8)
C18	0.0352 (8)	0.0455 (10)	0.0433 (9)	0.0007 (8)	0.0163 (7)	0.0050 (8)
C19	0.0380 (8)	0.0542 (11)	0.0494 (10)	−0.0012 (8)	0.0206 (7)	0.0113 (9)
C20	0.0346 (8)	0.0618 (11)	0.0409 (9)	0.0026 (8)	0.0167 (7)	0.0020 (9)
C21	0.0399 (8)	0.0511 (10)	0.0457 (10)	0.0012 (8)	0.0172 (7)	−0.0046 (9)
C22	0.0393 (8)	0.0464 (10)	0.0408 (9)	−0.0026 (8)	0.0158 (7)	0.0003 (8)

C23	0.0612 (10)	0.0472 (11)	0.0587 (11)	−0.0110 (9)	0.0269 (9)	−0.0012 (9)
C24	0.0755 (12)	0.0713 (14)	0.0990 (16)	−0.0283 (11)	0.0415 (12)	−0.0053 (13)
C25	0.1207 (16)	0.0698 (14)	0.0628 (13)	−0.0133 (13)	0.0443 (12)	0.0119 (11)
C26	0.1037 (15)	0.0477 (12)	0.1044 (17)	−0.0043 (12)	0.0532 (13)	−0.0026 (12)
C27	0.0565 (9)	0.0487 (11)	0.0801 (12)	0.0080 (9)	0.0392 (9)	0.0096 (10)
C28	0.1188 (16)	0.0573 (13)	0.0998 (16)	0.0070 (13)	0.0637 (13)	−0.0119 (12)
C29	0.0912 (13)	0.0477 (12)	0.1248 (17)	0.0076 (11)	0.0643 (12)	0.0154 (12)
C30	0.0632 (12)	0.0791 (15)	0.133 (2)	0.0299 (11)	0.0492 (12)	0.0286 (14)
C15	0.0585 (10)	0.0878 (15)	0.0508 (10)	0.0038 (10)	0.0283 (8)	−0.0017 (10)
O2	0.0523 (8)	0.0869 (11)	0.0372 (8)	0.0066 (8)	0.0153 (6)	0.0022 (8)
C16	0.0718 (16)	0.142 (3)	0.0366 (13)	0.0054 (17)	0.0159 (12)	0.0100 (15)
C15'	0.0585 (10)	0.0878 (15)	0.0508 (10)	0.0038 (10)	0.0283 (8)	−0.0017 (10)
O2'	0.043 (6)	0.204 (15)	0.049 (7)	0.037 (8)	0.006 (5)	−0.019 (8)
C16'	0.069 (6)	0.087 (7)	0.061 (6)	−0.005 (6)	0.029 (5)	−0.002 (6)
C31	0.0554 (9)	0.0890 (14)	0.0601 (10)	−0.0009 (10)	0.0362 (8)	0.0004 (10)
O4	0.0464 (7)	0.0904 (11)	0.0556 (8)	−0.0017 (8)	0.0326 (6)	0.0079 (8)
C32	0.0657 (12)	0.163 (3)	0.0771 (15)	−0.0018 (17)	0.0522 (11)	0.0131 (17)
C31'	0.0554 (9)	0.0890 (14)	0.0601 (10)	−0.0009 (10)	0.0362 (8)	0.0004 (10)
O4'	0.065 (4)	0.091 (4)	0.065 (4)	0.001 (3)	0.038 (3)	−0.001 (4)
C32'	0.061 (6)	0.073 (7)	0.066 (6)	0.012 (5)	0.048 (4)	0.001 (5)

Geometric parameters (Å, °)

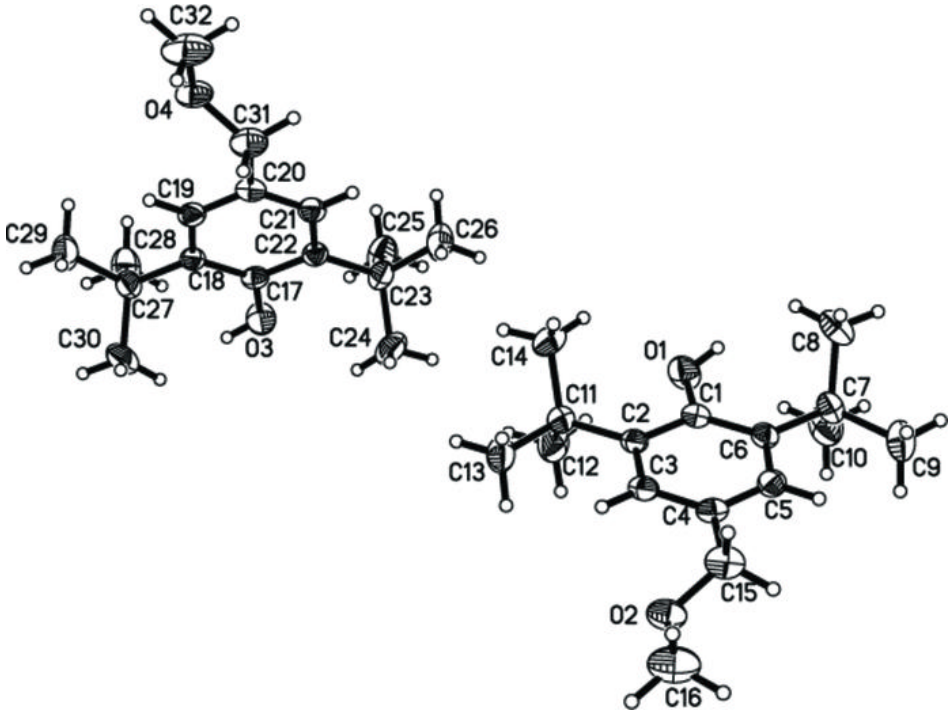
O1—C1	1.373 (2)	C21—H21	0.9300
O1—H1	0.8200	C22—C23	1.542 (3)
O3—C17	1.376 (2)	C23—C24	1.524 (3)
O3—H3	0.8200	C23—C26	1.534 (3)
C1—C6	1.400 (2)	C23—C25	1.534 (3)
C1—C2	1.410 (2)	C24—H24A	0.9600
C2—C3	1.386 (2)	C24—H24B	0.9600
C2—C11	1.539 (2)	C24—H24C	0.9600
C3—C4	1.378 (2)	C25—H25A	0.9600
C3—H3A	0.9300	C25—H25B	0.9600
C4—C5	1.372 (2)	C25—H25C	0.9600
C4—C15	1.511 (2)	C26—H26A	0.9600
C5—C6	1.388 (2)	C26—H26B	0.9600
C5—H5	0.9300	C26—H26C	0.9600
C6—C7	1.541 (3)	C27—C28	1.521 (3)
C7—C10	1.531 (4)	C27—C30	1.528 (3)
C7—C8	1.541 (3)	C27—C29	1.549 (3)
C7—C9	1.542 (3)	C28—H28A	0.9600
C8—H8A	0.9600	C28—H28B	0.9600
C8—H8B	0.9600	C28—H28C	0.9600
C8—H8C	0.9600	C29—H29A	0.9600
C9—H9A	0.9600	C29—H29B	0.9600
C9—H9B	0.9600	C29—H29C	0.9600
C9—H9C	0.9600	C30—H30A	0.9600
C10—H10A	0.9600	C30—H30B	0.9600
C10—H10B	0.9600	C30—H30C	0.9600

C10—H10C	0.9600	C15—O2	1.382 (2)
C11—C12	1.528 (3)	C15—H15A	0.9700
C11—C14	1.530 (3)	C15—H15B	0.9700
C11—C13	1.543 (3)	O2—C16	1.424 (3)
C12—H12A	0.9600	C16—H16A	0.9600
C12—H12B	0.9600	C16—H16B	0.9600
C12—H12C	0.9600	C16—H16C	0.9600
C13—H13A	0.9600	O2'—C16'	1.449 (8)
C13—H13B	0.9600	C16'—H16D	0.9600
C13—H13C	0.9600	C16'—H16E	0.9600
C14—H14A	0.9600	C16'—H16F	0.9600
C14—H14B	0.9600	C31—O4	1.383 (2)
C14—H14C	0.9600	C31—H31A	0.9700
C17—C18	1.403 (2)	C31—H31B	0.9700
C17—C22	1.404 (2)	O4—C32	1.429 (3)
C18—C19	1.396 (3)	C32—H32A	0.9600
C18—C27	1.529 (3)	C32—H32B	0.9600
C19—C20	1.374 (3)	C32—H32C	0.9600
C19—H19	0.9300	O4'—C32'	1.445 (9)
C20—C21	1.373 (3)	C32'—H32D	0.9600
C20—C31	1.507 (3)	C32'—H32E	0.9600
C21—C22	1.389 (3)	C32'—H32F	0.9600
C1—O1—H1	109.5	C24—C23—C26	106.94 (17)
C17—O3—H3	109.5	C24—C23—C25	110.1 (2)
O1—C1—C6	122.15 (15)	C26—C23—C25	107.30 (17)
O1—C1—C2	115.50 (15)	C24—C23—C22	110.80 (15)
C6—C1—C2	122.33 (15)	C26—C23—C22	111.50 (19)
C3—C2—C1	116.88 (16)	C25—C23—C22	110.07 (15)
C3—C2—C11	121.88 (15)	C23—C24—H24A	109.5
C1—C2—C11	121.24 (15)	C23—C24—H24B	109.5
C4—C3—C2	122.57 (16)	H24A—C24—H24B	109.5
C4—C3—H3A	118.7	C23—C24—H24C	109.5
C2—C3—H3A	118.7	H24A—C24—H24C	109.5
C5—C4—C3	118.45 (15)	H24B—C24—H24C	109.5
C5—C4—C15	118.95 (17)	C23—C25—H25A	109.5
C3—C4—C15	122.52 (17)	C23—C25—H25B	109.5
C4—C5—C6	123.06 (17)	H25A—C25—H25B	109.5
C4—C5—H5	118.5	C23—C25—H25C	109.5
C6—C5—H5	118.5	H25A—C25—H25C	109.5
C5—C6—C1	116.70 (16)	H25B—C25—H25C	109.5
C5—C6—C7	120.77 (16)	C23—C26—H26A	109.5
C1—C6—C7	122.53 (16)	C23—C26—H26B	109.5
C10—C7—C8	110.73 (19)	H26A—C26—H26B	109.5
C10—C7—C6	111.01 (18)	C23—C26—H26C	109.5
C8—C7—C6	109.59 (17)	H26A—C26—H26C	109.5
C10—C7—C9	107.1 (2)	H26B—C26—H26C	109.5
C8—C7—C9	107.01 (19)	C28—C27—C30	111.0 (2)
C6—C7—C9	111.29 (17)	C28—C27—C18	111.22 (16)
C7—C8—H8A	109.5	C30—C27—C18	110.47 (16)

C7—C8—H8B	109.5	C28—C27—C29	106.11 (18)
H8A—C8—H8B	109.5	C30—C27—C29	106.62 (17)
C7—C8—H8C	109.5	C18—C27—C29	111.22 (18)
H8A—C8—H8C	109.5	C27—C28—H28A	109.5
H8B—C8—H8C	109.5	C27—C28—H28B	109.5
C7—C9—H9A	109.5	H28A—C28—H28B	109.5
C7—C9—H9B	109.5	C27—C28—H28C	109.5
H9A—C9—H9B	109.5	H28A—C28—H28C	109.5
C7—C9—H9C	109.5	H28B—C28—H28C	109.5
H9A—C9—H9C	109.5	C27—C29—H29A	109.5
H9B—C9—H9C	109.5	C27—C29—H29B	109.5
C7—C10—H10A	109.5	H29A—C29—H29B	109.5
C7—C10—H10B	109.5	C27—C29—H29C	109.5
H10A—C10—H10B	109.5	H29A—C29—H29C	109.5
C7—C10—H10C	109.5	H29B—C29—H29C	109.5
H10A—C10—H10C	109.5	C27—C30—H30A	109.5
H10B—C10—H10C	109.5	C27—C30—H30B	109.5
C12—C11—C14	110.25 (18)	H30A—C30—H30B	109.5
C12—C11—C2	110.47 (17)	C27—C30—H30C	109.5
C14—C11—C2	111.54 (16)	H30A—C30—H30C	109.5
C12—C11—C13	107.62 (18)	H30B—C30—H30C	109.5
C14—C11—C13	106.10 (17)	O2—C15—C4	110.88 (17)
C2—C11—C13	110.70 (15)	O2—C15—H15A	109.5
C11—C12—H12A	109.5	C4—C15—H15A	109.5
C11—C12—H12B	109.5	O2—C15—H15B	109.5
H12A—C12—H12B	109.5	C4—C15—H15B	109.5
C11—C12—H12C	109.5	H15A—C15—H15B	108.1
H12A—C12—H12C	109.5	C15—O2—C16	111.31 (19)
H12B—C12—H12C	109.5	O2—C16—H16A	109.5
C11—C13—H13A	109.5	O2—C16—H16B	109.5
C11—C13—H13B	109.5	H16A—C16—H16B	109.5
H13A—C13—H13B	109.5	O2—C16—H16C	109.5
C11—C13—H13C	109.5	H16A—C16—H16C	109.5
H13A—C13—H13C	109.5	H16B—C16—H16C	109.5
H13B—C13—H13C	109.5	O2'—C16'—H16D	109.5
C11—C14—H14A	109.5	O2'—C16'—H16E	109.5
C11—C14—H14B	109.5	H16D—C16'—H16E	109.5
H14A—C14—H14B	109.5	O2'—C16'—H16F	109.5
C11—C14—H14C	109.5	H16D—C16'—H16F	109.5
H14A—C14—H14C	109.5	H16E—C16'—H16F	109.5
H14B—C14—H14C	109.5	O4—C31—C20	111.93 (17)
O3—C17—C18	121.74 (16)	O4—C31—H31A	109.2
O3—C17—C22	115.43 (16)	C20—C31—H31A	109.2
C18—C17—C22	122.82 (18)	O4—C31—H31B	109.2
C19—C18—C17	116.31 (16)	C20—C31—H31B	109.2
C19—C18—C27	121.06 (17)	H31A—C31—H31B	107.9
C17—C18—C27	122.61 (18)	C31—O4—C32	111.38 (19)
C20—C19—C18	122.59 (17)	O4—C32—H32A	109.5
C20—C19—H19	118.7	O4—C32—H32B	109.5

C18—C19—H19	118.7	H32A—C32—H32B	109.5
C21—C20—C19	119.02 (18)	O4—C32—H32C	109.5
C21—C20—C31	120.16 (18)	H32A—C32—H32C	109.5
C19—C20—C31	120.73 (18)	H32B—C32—H32C	109.5
C20—C21—C22	122.41 (17)	O4'—C32'—H32D	109.5
C20—C21—H21	118.8	O4'—C32'—H32E	109.5
C22—C21—H21	118.8	H32D—C32'—H32E	109.5
C21—C22—C17	116.82 (17)	O4'—C32'—H32F	109.5
C21—C22—C23	121.21 (17)	H32D—C32'—H32F	109.5
C17—C22—C23	121.97 (18)	H32E—C32'—H32F	109.5
O1—C1—C2—C3	179.52 (16)	C22—C17—C18—C27	179.76 (15)
C6—C1—C2—C3	1.3 (3)	C17—C18—C19—C20	0.5 (2)
O1—C1—C2—C11	−0.3 (3)	C27—C18—C19—C20	179.07 (15)
C6—C1—C2—C11	−178.52 (18)	C18—C19—C20—C21	0.9 (2)
C1—C2—C3—C4	−0.8 (3)	C18—C19—C20—C31	−175.59 (15)
C11—C2—C3—C4	179.05 (18)	C19—C20—C21—C22	−1.3 (2)
C2—C3—C4—C5	−0.3 (3)	C31—C20—C21—C22	175.23 (15)
C2—C3—C4—C15	176.40 (18)	C20—C21—C22—C17	0.2 (2)
C3—C4—C5—C6	1.0 (3)	C20—C21—C22—C23	−178.79 (15)
C15—C4—C5—C6	−175.84 (18)	O3—C17—C22—C21	−179.85 (14)
C4—C5—C6—C1	−0.5 (3)	C18—C17—C22—C21	1.4 (2)
C4—C5—C6—C7	178.64 (19)	O3—C17—C22—C23	−0.9 (2)
O1—C1—C6—C5	−178.78 (17)	C18—C17—C22—C23	−179.64 (15)
C2—C1—C6—C5	−0.7 (3)	C21—C22—C23—C24	117.6 (2)
O1—C1—C6—C7	2.1 (3)	C17—C22—C23—C24	−61.3 (2)
C2—C1—C6—C7	−179.83 (18)	C21—C22—C23—C26	−1.4 (2)
C5—C6—C7—C10	122.6 (2)	C17—C22—C23—C26	179.73 (15)
C1—C6—C7—C10	−58.3 (2)	C21—C22—C23—C25	−120.32 (19)
C5—C6—C7—C8	−114.8 (2)	C17—C22—C23—C25	60.8 (2)
C1—C6—C7—C8	64.4 (3)	C19—C18—C27—C28	122.42 (19)
C5—C6—C7—C9	3.4 (3)	C17—C18—C27—C28	−59.2 (2)
C1—C6—C7—C9	−177.5 (2)	C19—C18—C27—C30	−113.8 (2)
C3—C2—C11—C12	−118.3 (2)	C17—C18—C27—C30	64.6 (2)
C1—C2—C11—C12	61.5 (2)	C19—C18—C27—C29	4.4 (2)
C3—C2—C11—C14	118.7 (2)	C17—C18—C27—C29	−177.19 (16)
C1—C2—C11—C14	−61.5 (3)	C5—C4—C15—O2	−148.81 (18)
C3—C2—C11—C13	0.8 (3)	C3—C4—C15—O2	34.4 (3)
C1—C2—C11—C13	−179.37 (19)	C4—C15—O2—C16	−175.74 (19)
O3—C17—C18—C19	179.58 (14)	C21—C20—C31—O4	142.81 (16)
C22—C17—C18—C19	−1.7 (2)	C19—C20—C31—O4	−40.7 (2)
O3—C17—C18—C27	1.1 (2)	C20—C31—O4—C32	174.72 (17)

Fig. 1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