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(1*S**,4*S**,5*R**,8*R**)-4,8-Diphenyl-3,7-dioxabicyclo[3.3.0]octan-2-one

Thomas Gelbrich* and Michael B. Hursthouse

Department of Chemistry, University of Southampton, Highfield, Southampton SO17 1BJ, England

Correspondence e-mail: gelbrich@soton.ac.uk

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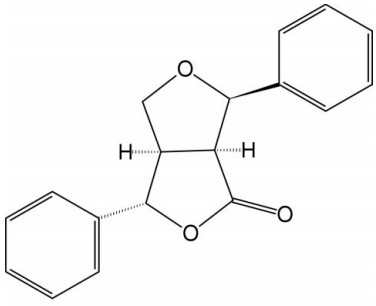
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.051
wR factor = 0.109
Data-to-parameter ratio = 12.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{18}H_{16}O_3$, (I), was prepared in the course of studies towards the synthesis of furofuran ligands and was reported previously [Brown & Hinks (1998). *Chem. Commun.* pp. 1895–1896]. The compound is a a model system, where both oxygenated aromatic rings that are present in the natural products have been substituted by a simple phenyl group.



(I)

Experimental

The furofuranone was recrystallized from Et_2O/hexanes as colourless crystals.

Crystal data

$C_{18}H_{16}O_3$
M_r = 280.31
Monoclinic, $C2/c$
a = 21.416 (1) Å
b = 7.520 (1) Å
c = 19.487 (1) Å
β = 117.86 (1)°
V = 2774.7 (3) Å^3
Z = 8
D_x = 1.342 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8593 reflections
θ = 2.9–25.2°
μ = 0.09 mm^{-1}
T = 150 (2) K
Block, colourless
0.30 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans to fill Ewald sphere
Absorption correction: multi-scan (Blessing, 1997)
T_{min} = 0.973, T_{max} = 0.987
7164 measured reflections
2489 independent reflections
1822 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 25.3°
$h = -24 \rightarrow 25$
$k = -9 \rightarrow 8$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.109
S = 0.97
2489 reflections
207 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0009P)^2 + 5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0062 (5)

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Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1990).

References

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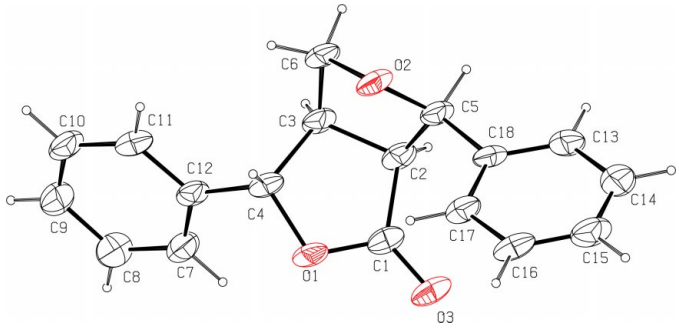

Figure 1
The structure of (I) showing 50% probability displacement ellipsoids.