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2,6-Diphenylthiapyran-4-one

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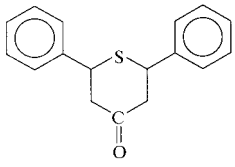
In the title compound, 2,6-diphenylthiacyclohexan-4-one, $C_{17}H_{16}OS$, mirror site symmetry is retained by the molecule in the solid state in the absence of C—H···*X* hydrogen bonds. The crystal structure is stabilized by van der Waals interactions, the shortest S···O and C···O contacts being 3.567 (2) and 3.512 (3) Å, respectively.

Comment

The tendency of molecules to pack as closely as possible usually overrides that for retention of molecular symmetry upon crystallization, and reduces the symmetry of a molecule in the solid state compared to that observed in the free state (Kitaigorodskii, 1973). Though inversion generally is the symmetry element which is carried over into the crystal, the tendency of molecules to possess mirror or twofold symmetry in the solid state seems to depend on the presence, nature and strength of the intermolecular interactions. An example of this is the crystal structure of 2,6-dibenzoyl-1,4-benzoquinone (Biradha *et al.*, 1997), where interference from numerous C—H···O hydrogen bonds lowers the symmetry of the molecule.



(I)

In the present structure, (I), the molecule is bisected by a mirror plane passing through atoms S1, C4 and O1 of the heterocyclic ring (Fig. 1). There are no C—H···*X*-type interactions whose presence otherwise might have had a considerable influence on the molecular conformation. The absence of C—H···O hydrogen bonds is presumably due to the deficiency of acceptors compared to donors (phenyl C—H). The crystal structure is stabilized by van der Waals interactions. The shortest S···O and C···O contacts observed are 3.567 (2) and 3.512 (3) Å, respectively. The structure provides a good example of the retention of mirror symmetry by a molecule in the crystal state.

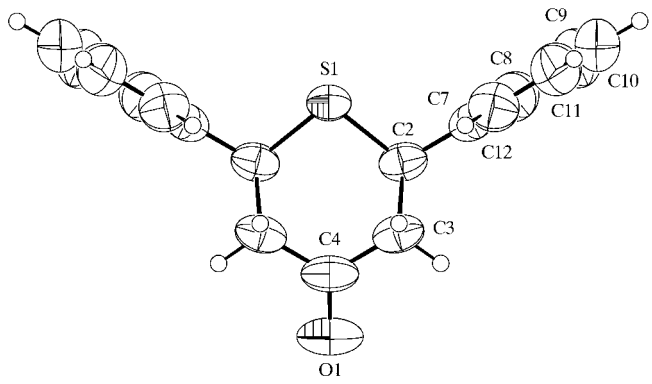


Figure 1
The molecular structure of (I) with the atom-numbering scheme and 50% probability displacement ellipsoids.

Experimental

Crystals of (I) were grown by slow evaporation of a saturated ethanol solution.

Crystal data

$C_{17}H_{16}OS$
M_r = 268.36
Orthorhombic, *Pnma*
a = 10.867 (3) Å
b = 24.284 (4) Å
c = 5.427 (2) Å
V = 1432.2 (7) Å^3
Z = 4
D_x = 1.245 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 8–16°
μ = 1.903 mm^{-1}
T = 293 (2) K
Plate, colourless
0.20 × 0.12 × 0.08 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
1585 measured reflections
1436 independent reflections
1285 reflections with $I > 2\sigma(I)$
R_{int} = 0.007
θ_{max} = 71.88°
$h = 0 \rightarrow 13$
$k = -29 \rightarrow 11$
$l = -6 \rightarrow 0$
2 standard reflections
every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
$R(F)$ = 0.043
$wR(F^2)$ = 0.123
S = 1.167
1436 reflections
124 parameters
H atoms refined isotropically
$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.1515P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.352 e Å^{-3}
$\Delta\rho_{min}$ = −0.179 e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.0126 (9)

Data collection, cell refinement and data reduction: *CAD*-4 *Software* (Enraf–Nonius, 1989); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLUTO* (Motherwell & Clegg, 1978); software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: VJ1103). Services for accessing these data are described at the back of the journal.

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