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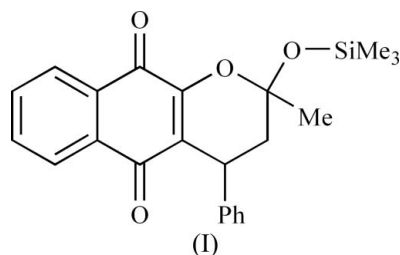
## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.056  
 $wR$  factor = 0.156  
Data-to-parameter ratio = 16.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.2-Methyl-4-phenyl-2-(trimethylsilyloxy)-3,4-dihydro-2H-naphtho[2,3-*b*]pyran-5,10-dioneReceived 1 July 2006  
Accepted 19 September 2006

In the title compound,  $\text{C}_{23}\text{H}_{24}\text{O}_4\text{Si}$ , the naphthalene ring system is essentially planar. The conformation of the dihydropyran ring is very similar to a half-chair form. There are intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions and  $\pi-\pi$  stacking interactions in the crystal structure.

## Comment

*o*-Quinone methides constitute a class of highly reactive intermediates and their cycloaddition chemistry has attracted considerable interest (Nair *et al.*, 2001). In our ongoing studies on the cycloaddition reactions of *o*-quinone methides, we have prepared the title compound, (I), which is obtained from the cycloaddition reaction between *o*-quinone methides derived from 2-hydroxy-1,4-naphthoquinone and an excess amount of trimethyl[(1-methylethenyl)oxy]silane. As part of this study, we have undertaken the X-ray crystallographic analysis of (I) in order to elucidate the conformation and configuration of this cycloadduct product.



The bond lengths and angles in (I) (Fig. 1) are in good agreement with expected values (Allen *et al.*, 1987). The phenyl ring at C7 is pseudo-axial to the pyran ring. The conformation of the pyran ring is very similar to a half-chair form.

The naphthalene ring system is essentially planar, with atom C14 deviating from the mean plane by 0.140 (4) Å. The dihedral angle between the naphthalene ring system and the phenyl ring C8–C13 is 76.8 (2)°.

In the crystal structure, no classical hydrogen bonds were found, but there is an intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interaction (Table 1). The crystal packing is also stabilized by  $\pi-\pi$  stacking interactions (Table 2) between neighbouring naphthoquinone units.

## Experimental

Under argon, a mixture of 2-hydroxy-1,4-naphthoquinone, 3 equivalents of trimethyl[(1-methylethenyl)oxy]silane and an excess amount of benzaldehyde were suspended in dry dioxane and refluxed

for about 20 h. Compound (I) was isolated in 24% yield by column chromatography of the reaction mixture on silica gel after evaporation of the solvent. Single crystals of (I) were obtained by slow evaporation of a petroleum ether–ethyl acetate (3:1 v/v) solution of (I).

#### Crystal data

$C_{23}H_{24}O_4Si$   
 $M_r = 392.51$   
 Monoclinic,  $P2_1/c$   
 $a = 12.699$  (3) Å  
 $b = 11.342$  (2) Å  
 $c = 15.023$  (3) Å  
 $\beta = 92.44$  (3)°  
 $V = 2161.8$  (8) Å<sup>3</sup>

#### Data collection

Enraf–Nonius CAD-4  
 diffractometer  
 $\omega/2\theta$  scans  
 Absorption correction:  $\psi$  scan  
 (XCAD4; Harms & Wocadlo, 1995)  
 $T_{\min} = 0.932$ ,  $T_{\max} = 0.957$   
 4407 measured reflections

$Z = 4$   
 $D_x = 1.206$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.13$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, colourless  
 0.40 × 0.35 × 0.33 mm

4215 independent reflections  
 2140 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.035$   
 $\theta_{\text{max}} = 26.0^\circ$   
 3 standard reflections  
 every 200 reflections  
 intensity decay: none

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.056$   
 $wR(F^2) = 0.156$   
 $S = 1.00$   
 4215 reflections  
 253 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 1P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.18$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.28$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$       | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------|-------|-------------|-------------|---------------|
| $C1-H1A\cdots O4^i$ | 0.96  | 2.47        | 3.343 (5)   | 151           |

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

**Table 2**

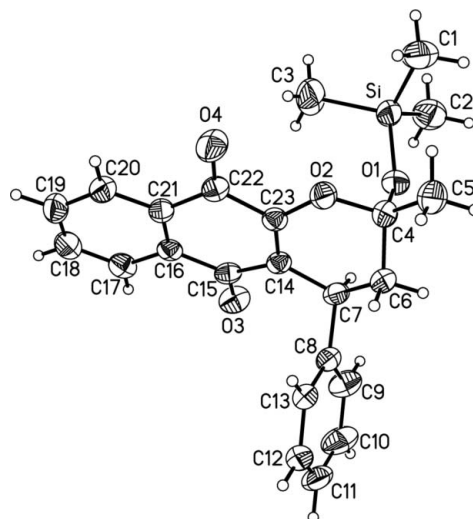
$\pi$ - $\pi$  interactions (Å, °).

| $CgI$ | $CgJ$ | Symmetry code   | $Cg\cdots Cg$ | Dihedral angle | Interplanar distance | Offset |
|-------|-------|-----------------|---------------|----------------|----------------------|--------|
| A     | A     | $-x, 2 - y, -z$ | 3.868 (2)     | 0.0 (2)        | 3.358 (3)            | 1.92   |

$Cg(A)$  denotes the centroid of the aromatic ring C16–C21. The offset is defined as the distance between  $Cg(I)$  and the perpendicular projection of  $Cg(J)$  on ring  $I$ .

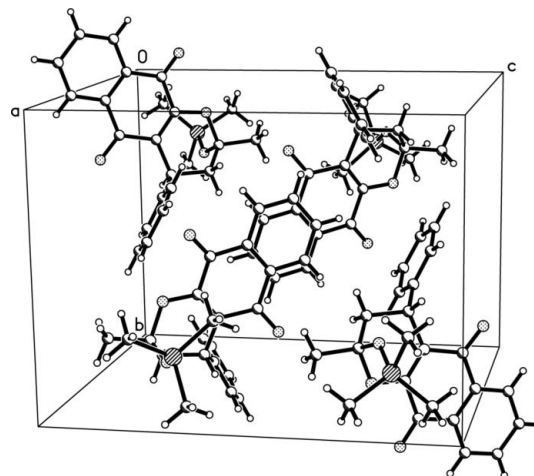
H atoms were included in the riding-model approximation, with  $C-H = 0.93, 0.96, 0.97$  and  $0.98$  Å for aromatic, methyl, methylene and methine H atoms, respectively, and with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(\text{aromatic, methylene and methine C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ .

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).



**Figure 1**

The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.



**Figure 2**

The crystal packing of (I), viewed approximately down the  $a$  axis.

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