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The crystal structure of 2-(2-methyl-6-phenyl-4*H*-pyran-4-ylidene)-1*H*-indene-1,3(2*H*)-dione, $C_{21}H_{14}O_3$

Table 1: Data collection and handling.

Crystal:	Colorless prismatic
Size:	0.20 × 0.17 × 0.11 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.09 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	25.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	10,546, 2827, 0.036
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1906
$N(\text{param})_{\text{refined}}$:	219
Programs:	Bruker [1], SHELX [2, 3], Diamond [4]

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Abstract

$C_{21}H_{14}O_3$, monoclinic, $P2_1/c$ (no. 14), $a = 4.8318(8)$ Å, $b = 26.590(4)$ Å, $c = 11.821(2)$ Å, $\beta = 91.050(4)^\circ$, $V = 1518.4(4)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0401$, $wR_{\text{ref}}(F) = 0.1038$, $T = 296(2)$ K.

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The molecular structure is shown in the figure (H atoms are omitted for clarity). Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was prepared according to the synthetic method reported in the previous literature [5].

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Crystals were obtained by slow evaporation from a mixture of ethyl acetate and ethanol.

Experimental details

H atoms were positioned geometrically and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2 U_{\text{eq}}(\text{C})$ for all other H atoms. All the non-hydrogen atoms were refined anisotropically.

Comment

The 4*H*-pyran unit has been demonstrated to be an excellent building block for constructing various organic fluorescent materials in the field of fluorescence sensors, security systems, and optical information storage [6, 7]. Furthermore, the researchers have also found that the intermolecular interactions and stacking arrangements often exhibit a very important influence on the photophysical properties of the materials [8]. Therefore, the investigation on the crystal structures of 4*H*-pyran derivatives has received wide attention [9–11].

In the title structure the 1*H*-indene-1,3(2*H*)-dione moiety and the 4*H*-pyran ring are almost in the same plane. The dihedral angle between the 4*H*-pyran ring and phenyl ring is determined to be 22.4°. This result indicates that the asymmetric molecule has a twisted molecular conformation,

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
O1	0.3744 (3)	0.69856 (5)	0.28643 (11)	0.0586 (4)
O2	0.3799 (3)	0.58705 (5)	−0.02697 (11)	0.0570 (4)
O3	1.0774 (3)	0.54301 (5)	0.30595 (10)	0.0456 (3)
C1	0.3227 (4)	0.67650 (7)	0.19703 (15)	0.0429 (4)
C2	0.1111 (4)	0.69327 (7)	0.11098 (15)	0.0431 (5)
C3	−0.0723 (4)	0.73308 (7)	0.11287 (18)	0.0541 (5)
H3	−0.0803	0.7543	0.1753	0.065*
C4	−0.2443 (4)	0.74058 (8)	0.0190 (2)	0.0618 (6)
H4	−0.3686	0.7673	0.0186	0.074*
C5	−0.2342 (4)	0.70904 (8)	−0.07387 (19)	0.0611 (6)
H5	−0.3503	0.7150	−0.1360	0.073*
C6	−0.0529 (4)	0.66870 (8)	−0.07529 (16)	0.0540 (5)
H6	−0.0465	0.6472	−0.1373	0.065*
C7	0.1183 (4)	0.66127 (7)	0.01821 (15)	0.0432 (5)
C8	0.3279 (4)	0.62090 (7)	0.04012 (15)	0.0423 (5)
C9	0.4515 (4)	0.63068 (7)	0.15223 (14)	0.0394 (4)
C10	0.6583 (4)	0.60203 (7)	0.20438 (14)	0.0384 (4)
C11	0.7664 (4)	0.55744 (7)	0.15314 (15)	0.0435 (5)
H11	0.6961	0.5475	0.0829	0.052*
C12	0.9650 (4)	0.52973 (7)	0.20296 (15)	0.0433 (5)
C13	0.9838 (4)	0.58547 (7)	0.35889 (14)	0.0403 (4)
C14	0.7813 (4)	0.61401 (7)	0.31254 (14)	0.0420 (4)
H14	0.7197	0.6421	0.3515	0.050*
C15	1.1289 (4)	0.59319 (7)	0.46811 (14)	0.0417 (4)
C16	1.2577 (4)	0.55315 (8)	0.52314 (16)	0.0553 (5)
H16	1.2550	0.5214	0.4900	0.066*
C17	1.3896 (5)	0.55996 (9)	0.62656 (17)	0.0668 (6)
H17	1.4735	0.5328	0.6628	0.080*
C18	1.3978 (5)	0.60674 (9)	0.67637 (17)	0.0647 (6)
H18	1.4854	0.6112	0.7464	0.078*
C19	1.2755 (5)	0.64668 (9)	0.62188 (17)	0.0659 (6)
H19	1.2823	0.6784	0.6549	0.079*
C20	1.1419 (5)	0.64027 (8)	0.51812 (16)	0.0563 (6)
H20	1.0606	0.6677	0.4819	0.068*
C21	1.0929 (5)	0.48308 (7)	0.15918 (17)	0.0571 (6)
H21A	0.9887	0.4714	0.0945	0.086*
H21B	1.0930	0.4577	0.2170	0.086*
H21C	1.2798	0.4899	0.1377	0.086*

which causes that no obvious $\pi\cdots\pi$ interactions are observed. Similar results can be found in previously reported structures of related 4*H*-pyran derivatives [5, 9, 11]. The molecules are linked by one kind of C20–H20 $\cdots\pi$ (benzene ring) bond with a distance of 3.570 Å and one kind of C21–H21A $\cdots$ O2 hydrogen bond with a distance of 2.484 Å.

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