

Dimethyl 2,2'-[(4-oxo-2-phenyl-4H-chromene-5,7-diyloxy]diacetate: a more densely packed polymorph

Angannan Nallasivam,^a Munirathinam Nethaji,^b Nagarajan Vembu,^{c*} Buckle Jaswant^d and Nagarajan Sulochana^a

^aDepartment of Chemistry, National Institute of Technology, Tiruchirappalli 620 015, India, ^bDepartment of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560 012, India, ^cDepartment of Chemistry, Urumu Dhanalakshmi College, Tiruchirappalli 620 019, India, and ^dDepartment of Chemistry, Government Arts College, Karur 639 005, India
Correspondence e-mail: vembu57@yahoo.com

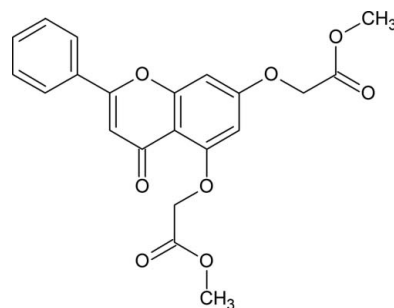
Received 11 November 2008; accepted 8 January 2009

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; disorder in main residue; R factor = 0.059; wR factor = 0.118; data-to-parameter ratio = 14.1.

The title molecule, $\text{C}_{21}\text{H}_{18}\text{O}_8$, crystallizes in two crystal polymorphs, see also Nallasivam, Nethaji, Vembu & Jaswant [*Acta Cryst.* (2009), **E65**, o314–o315]. The molecules of both polymorphs differ by the conformation of the oxomethylacetate groups. The title molecules are rather planar compared to the molecules of the other polymorph. In the title molecule, one of the oxomethylacetate groups is disordered (occupancies of 0.6058/0.3942). The structures of both polymorphs are stabilized by $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\pi$ interactions. Due to the planarity of the title molecules and similar intermolecular interactions, the title molecules are more densely packed than those of the other polymorph.

Related literature

For a more detailed description of the two polymorphs, see: Nallasivam *et al.* (2009). For related structures, see: Wang, Fang *et al.* (2003); Wang, Zheng *et al.* (2003). For hydrogen bonding, see: Desiraju & Steiner (1999).



Experimental

Crystal data

$\text{C}_{21}\text{H}_{18}\text{O}_8$
 $M_r = 398.35$
Triclinic, $P\bar{1}$
 $a = 7.4290$ (15) Å
 $b = 9.2582$ (19) Å
 $c = 13.480$ (3) Å
 $\alpha = 84.232$ (3)°
 $\beta = 88.775$ (4)°
 $\gamma = 82.982$ (3)°
 $V = 915.5$ (3) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹
 $T = 293$ (2) K
0.34 × 0.28 × 0.22 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
 $T_{\min} = 0.963$, $T_{\max} = 0.975$
9755 measured reflections
3781 independent reflections
2887 reflections with $I > 3\sigma(I)$
 $R_{\text{int}} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$
 $wR(F^2) = 0.118$
 $S = 2.47$
3781 reflections
268 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.40$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C8}-\text{H8}\cdots\text{O27}^i$	0.93	2.38	3.304 (2)	169
$\text{C12}-\text{H12}\cdots\text{O1}$	0.93	2.33	2.664 (2)	101
$\text{C15}-\text{H15}\cdots\text{O21B}^{ii}$	0.93	2.46	3.31 (6)	153
$\text{C25}-\text{H25B}\cdots\text{O17}^{iii}$	0.97	2.56	3.447 (3)	153
$\text{C29}-\text{H29B}\cdots\text{O17}^{iv}$	0.96	2.50	3.403 (3)	156
$\text{C29}-\text{H29C}\cdots\text{O21B}^{iv}$	0.96	2.55	3.26 (6)	131
$\text{C23B}-\text{H23BB}\cdots\text{Cg1}^v$	0.96	2.76	3.67 (6)	159 (6)

Symmetry codes: (i) $-x, -y + 3, -z + 2$; (ii) $-x + 1, -y + 1, -z + 2$; (iii) $x, y + 1, z$; (iv) $x - 1, y + 1, z$; (v) $x, y, z - 1$. Cg1 is the centroid of the C11–C16 phenyl ring.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *JANA2000* (Petříček *et al.*, 2000); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *JANA2000*.

AN thanks Dr Naresh Kumar and Dr G. Vengatachalam, School of Chemistry, Bharathidasan University, Tiruchirappalli, and Organica Aromatics Pvt Ltd, Bangalore, India, for providing laboratory facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FB2129).

References

- Bruker (1999). *SMART* and *SAINT*. Bruker AXS Inc, Madison, Wisconsin, USA.
- Desiraju, G. R. & Steiner, T. (1999). *The Weak Hydrogen Bond in Structural Chemistry and Biology*. New York: Oxford University Press.
- Nallasivam, A., Nethaji, M., Vembu, N., Jaswant, B. & Sulochana, N. (2009). *Acta Cryst.* **E65**, o314–o315.
- Petríček, V., Dušek, M. & Palatinus, L. (2000). *JANA2000*. Institute of Physics, Czech Academy of Science, Czech Republic.
- Sheldrick, G. M. (1998). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Wang, J.-F., Fang, M.-J., Huang, H.-Q., Li, G.-L., Su, W.-J. & Zhao, Y.-F. (2003). *Acta Cryst.* **E59**, o1517–o1518.
- Wang, J.-F., Zhang, Y.-J., Fang, M.-J., Huang, Y.-J., Wei, Z.-B., Zheng, Z.-H., Su, W.-J. & Zhao, Y.-F. (2003). *Acta Cryst.* **E59**, o1244–o1245.