Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

1,3-Dipropionyl-2,4,6-trimethylbenzene

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Received 5 December 2006
Accepted 8 December 2006

Key indicators

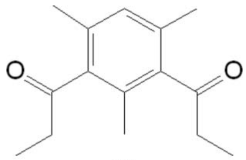
Single-crystal X-ray study
T = 110 K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.093
Data-to-parameter ratio = 8.8

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

In the molecule of the title compound, $C_{15}H_{20}O_2$, the two propionyl groups are in unusual positions with the two carbonyl groups in *syn* orientation relative to each other and bent at angles of 94.3 (3) and 93.6 (2)° away from the central methyl group.

Comment

In a previous study, involving orientation of carbonyl groups by adjacent methyls (Pinkus *et al.*, 2006), dipropiodurene [systematic name: 1,1′-(2,3,5,6-tetramethyl-*p*-phenylene)dipropan-1-one] was found to have a *trans* orientation relative to the central ring with the planes of the carbonyl group and attached methylene C atom at a dihedral angle of 86.50 (11)° relative to the central ring. In a related crystallographic study of 1,4-bis(4-chlorobenzoyl)-2,3,5,6-tetramethylbenzene by Ferguson *et al.* (1993), it was reported that the two *p*-chlorobenzoyl groups were also in a *trans* orientation, with a corresponding angle of 85.9 (1)°. Casarini & Lunazzi (1996) separated orthogonal *syn*/*anti* isomers of 1,4-bis(2,2-dimethyl propanoyl)durene by preparative TLC. In a more recent study Coluccini *et al.* (2003) observed more complicated rotamers in both *syn* and *anti* forms of 1,4-bis(mesitoyl)-2,3,5,6-tetramethylbenzene in low temperature NMR spectra. It was of interest to examine the related angles in the molecule of the title compound, (I), for which *syn*/*anti* orientations of keto groups are also possible.


(I)

In the molecule of (I) (Fig. 1) the bond lengths and angles (Table 1) are within expected ranges. The two propionyl groups are in unusual positions with the two carbonyl groups in *syn* orientation relative to each other and bent at angles of 94.3 (3) and 93.6 (2)° away from the central C7 methyl group.

Experimental

Dipropionylmesitylene was prepared (yield 79%; m.p. 373–374 K, literature 374–375 K) according to a previously reported procedure (Weil, 1897). Crystals suitable for X-ray analysis were obtained from absolute ethanol.

Crystal data

$C_{15}H_{20}O_2$
$M_r = 232.31$
Monoclinic, *Cc*
$a = 7.9058$ (10) Å
$b = 21.191$ (3) Å
$c = 8.8305$ (13) Å
$\beta = 111.989$ (4)°
$V = 1371.8$ (3) $Å^3$
$Z = 4$
$D_x = 1.125$ Mg m^{-3}
Mo *Kα* radiation
$\mu = 0.07$ mm^{-1}
$T = 110$ (2) K
Block, colorless
0.32 × 0.25 × 0.21 mm

Data collection

Bruker X8 APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.977$, $T_{max} = 0.985$
6948 measured reflections
1399 independent reflections
1336 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 26.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.093$
$S = 1.07$
1399 reflections
159 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.257P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e $Å^{-3}$
$\Delta\rho_{min} = -0.16$ e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

O1—C10	1.210 (2)	C6—C13	1.503 (3)
O2—C13	1.207 (2)	C10—C11	1.502 (3)
C2—C10	1.505 (3)	C14—C13	1.504 (3)
O1—C10—C11	121.89 (18)	O2—C13—C6	121.42 (17)
O1—C10—C2	120.94 (18)	O2—C13—C14	122.52 (18)
C11—C10—C2	117.16 (16)	C6—C13—C14	116.06 (16)

H atoms were positioned geometrically, with C—H = 0.95, 0.99 and 0.98 Å for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.5$ for methyl and $x = 1.2$ for all other H atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *APEX2* (Bruker, 2003); cell refinement: *APEX2*; data reduction: *SAINT-Plus* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

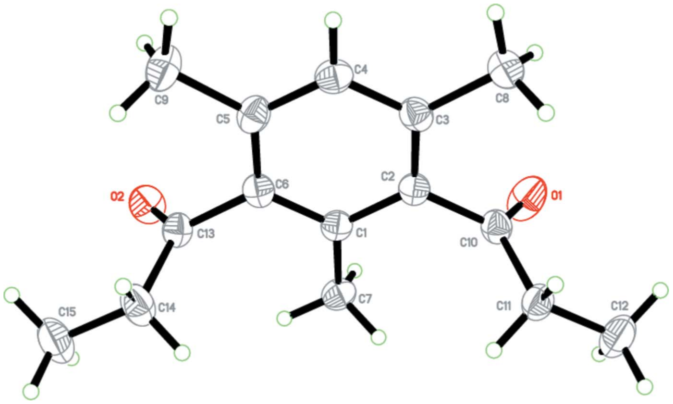


Figure 1
A view of the molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

The Bruker X8 APEX diffractometer was purchased with funds received from the National Science Foundation Major Research Instrumentation Program, grant No. CHE-0321214. KKK and AGP thank the Robert A. Welch Foundation for support (grant Nos. AA-1508 and AA-111, resectively).

References

Bruker (2003). *APEX2* (Version 2.0) and *SAINT-Plus* (Version 6.25). Bruker AXS Inc., Madison, Wisconsin, USA.
Casarini, D. & Lunazzi, L. (1996). *J. Org. Chem.* **61**, 6240–6243.
Coluccini, C., Grilli, S. & Mazzanti, A. (2003). *J. Org. Chem.* **68**, 7266–7273.
Ferguson, G., Patterson, K. H. & Smith, D. M. (1993). *Acta Cryst.* C**49**, 190–192.
Pinkus, A. G., Klausmeyer, K. K., Carson, C. E. & Custard, H. C. (2006). *Acta Cryst.* E**62**, o1854–o1855.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Weil, H. (1897). *Chem. Ber.* **30**, 1285–1286.

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