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(*E*)-2,2,6,6-Tetramethylhept-4-en-3-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.098
Data-to-parameter ratio = 17.1

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

The title compound, $C_{11}H_{20}O$, shows a wide $Me_3C-C{=}C$ angle of 129.60 (14)°. Molecules associate into zigzag chains parallel to [101] *via* a hydrogen bond $H_{methyl}\cdots O_{ketone}$.

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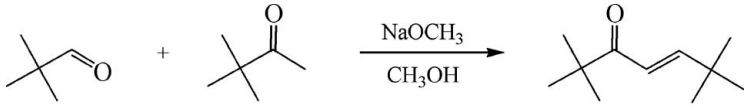
Comment

In our studies of the stereochemistry, stability and chemical properties of *tert*-butylated oligo- and polyolefins (Hopf *et al.*, 1998), we prepared a sample of the title compound, (3), a known α,β-unsaturated ketone (Dimroth & Mach, 1968). We present here its structure.



(1) (2) (3) (~46%)

The molecule is shown in Fig. 1. Bond lengths and angles, *e.g.* the C=C bond length of 1.325 (2) Å, may be regarded as normal. The angle C4=C5—C6 is widened to 129.60 (14)°, but this is normal for the ^{t}Bu—CH=C group; a search of the Cambridge Structural Database (Version 5.26; Allen, 2002) gave 42 examples of this fragment with a mean angle of 129.7°. Atoms C2–C6 and C11 are coplanar within an r.m.s. deviation of 0.009 Å. Atom C8 lies only 0.111 (2) Å out of this plane.

The crystal packing involves only one significant contact, the hydrogen bond C10—H10···O1($-\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$), which is long but of acceptable linearity. This links the molecules to form zigzag chains with overall direction [101] (Fig. 2).

Experimental

Compound (3) was prepared by base-catalyzed condensation of 2,2-dimethylpropanal, (1), with 3,3-dimethyl-2-butanone, (2), as

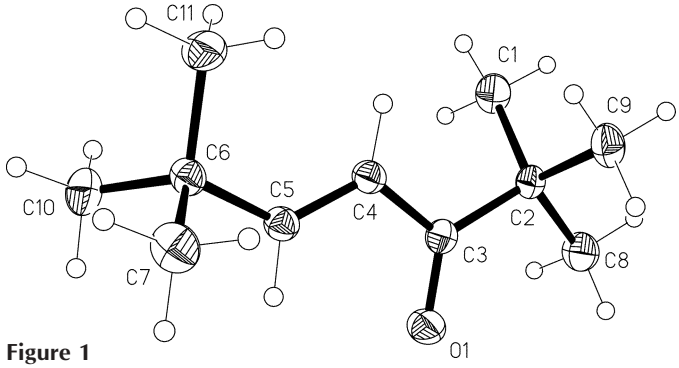


Figure 1
The molecule of the title compound in the crystal structure. Displacement ellipsoids are drawn at the 30% probability level.

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described by Dimroth & Mach (1968). Single crystals were obtained by sublimation.

Crystal data

$C_{11}H_{20}O$
M_r = 168.27
Monoclinic, $P2_1/n$
a = 5.8205 (5) Å
b = 18.0795 (15) Å
c = 10.6725 (10) Å
β = 94.324 (6)°
V = 1119.89 (17) Å^3
Z = 4
D_x = 0.998 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 63 reflections
θ = 4–12.5°
μ = 0.06 mm^{-1}
T = 173 (2) K
Prism, colourless
0.7 × 0.5 × 0.4 mm

Data collection

Siemens P4 diffractometer
ω scans
Absorption correction: none
2161 measured reflections
1961 independent reflections
1262 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.0°
$h = 0 \rightarrow 6$
$k = 0 \rightarrow 21$
$l = -12 \rightarrow 12$
3 standard reflections
every 247 reflections
intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.098
S = 0.93
1961 reflections
115 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C2—C3	1.524 (2)	C4—C5	1.325 (2)
C3—C4	1.484 (2)	C5—C6	1.501 (2)
O1—C3—C4	120.38 (14)	C4—C3—C2	118.80 (13)
O1—C3—C2	120.81 (14)	C4—C5—C6	129.60 (14)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10B···O1^{i}	0.98	2.65	3.615 (2)	169

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

Methyl H atoms were identified in difference syntheses, idealized and then refined using rigid methyl groups (C—H = 0.98 Å and H—C—H = 109.5°) allowed to rotate but not tip. Other H atoms were included using a riding model, with C—H = 0.95 Å. U_{iso}(H) values were fixed at 1.2U_{eq} of the parent atom.

Data collection: *XSCANS* (Fait, 1991); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP5* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

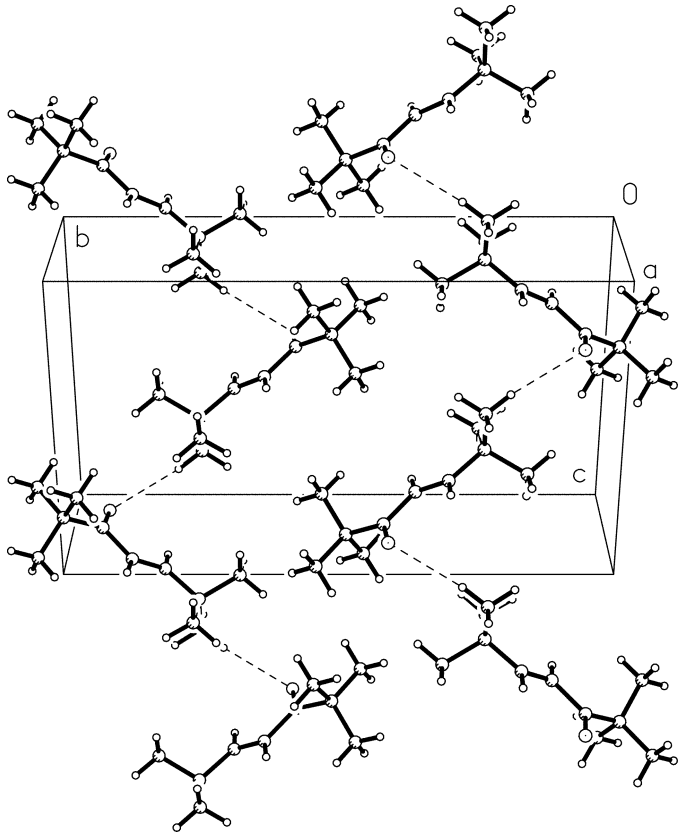

Figure 2
Packing diagram of the title compound viewed perpendicular to the plane (10$\bar{1}$). Hydrogen bonds are indicated by dashed bonds.

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