Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,7-Dimethylocta-2,3,5,6-tetraene

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Key indicators

Single-crystal X-ray study
T = 178 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.121
Data-to-parameter ratio = 14.0

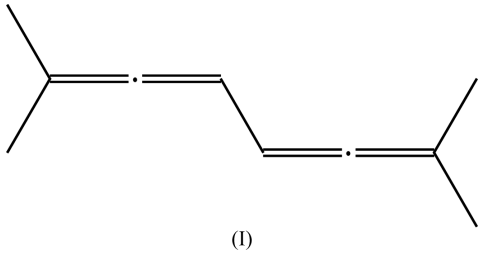
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 4 February 2002
Accepted 7 February 2002
Online 22 February 2002

The molecule of the title compound, $C_{10}H_{14}$, displays inversion symmetry. The allenic bond lengths are 1.3067 (16) and 1.3126 (16) Å.

Comment

Conjugated bis-allenes are interesting starting materials in organic chemistry and have been used, in particular, as diene components in Diels–Alder addition (for a summary, see Hopf, 2000). In a study of the behaviour of bis-allenes in ionic reaction, we have prepared one of the oldest known bis-allenes, the title compound 2,7-dimethyl-octa-2,3,5,6-tetraene, (I) (Skattebøl & Solomon, 1965), and subjected it to structure determination.



(I)

The molecule (Fig. 1) displays crystallographic inversion symmetry, because of which the standard IUPAC numbering was not used. Molecular dimensions may be regarded as normal [*cf. e.g.* the standard allenic C=C bond length of 1.307 Å (Allen *et al.*, 1987)]. The allenic angle C2—C4—C5 is essentially linear at 179.89 (13)° and the angle C4—C5—C5^{i} 124.04 (13)° somewhat wider than the standard sp^2 value [symmetry code: (i) 1−*x*, 1−*y*, −*z*]. The shortest intermolecular contact is H1*A*···H1*C*(−0.5+*x*, 0.5−*y*, −0.5+*z*), 2.55 (2) Å, and the molecules pack in the common herringbone pattern (Fig. 2).

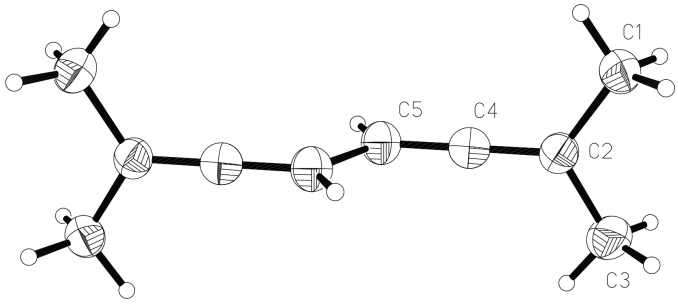


Figure 1
The molecule of the title compound in the crystal. Ellipsoids represent 50% probability levels.

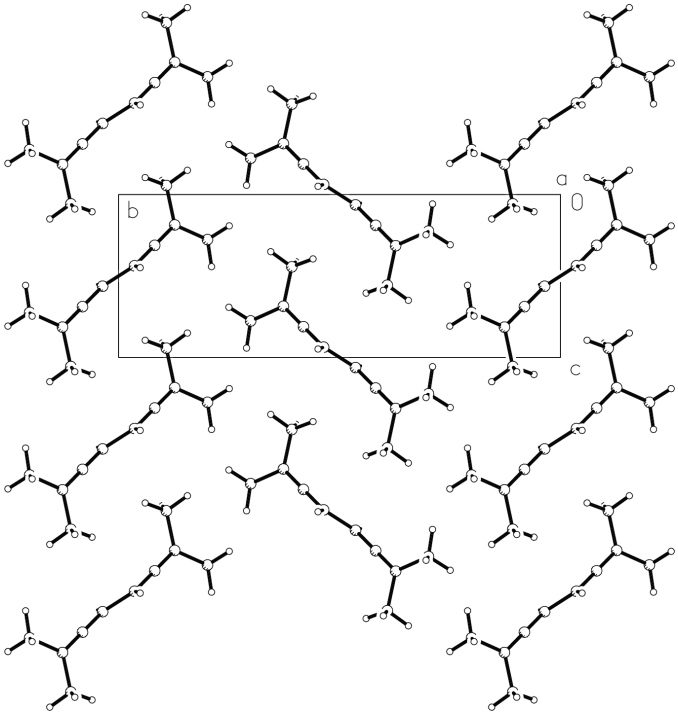


Figure 2
Packing diagram of the title compound, projected along the *a* axis. Radii are arbitrary.

Experimental

Crystals were grown by sublimation.

Crystal data

$C_{10}H_{14}$
M_r = 134.21
Monoclinic, $P2_1/n$
a = 4.644 (2) Å
b = 16.278 (6) Å
c = 6.037 (2) Å
β = 96.12 (3)°
V = 453.8 (3) Å^3
Z = 2
D_x = 0.982 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 50 reflections
θ = 10–12.5°
μ = 0.06 mm^{-1}
T = 178 (2) K
Prism, colourless
0.70 × 0.25 × 0.25 mm

Data collection

Nicolet $R3$ diffractometer
ω scans
Absorption correction: none
2589 measured reflections
1034 independent reflections
810 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.5°
$h = -5 \rightarrow 6$
$k = -21 \rightarrow 21$
$l = -7 \rightarrow 7$
3 standard reflections
every 147 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.121
S = 1.06
1034 reflections
74 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2 + 0.0479P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.5076 (17)	C4—C5	1.3126 (16)
C2—C4	1.3067 (16)	C5—C5^{i}	1.470 (2)
C2—C3	1.5067 (17)		
C4—C2—C3	122.22 (11)	C2—C4—C5	179.89 (13)
C4—C2—C1	121.93 (10)	C4—C5—C5^{i}	124.04 (13)
C3—C2—C1	115.85 (10)		

Symmetry code: (i) $1-x, 1-y, -z$.

A rigid-body libration correction (Schomaker & Trueblood, 1968) was performed successfully (R_{lib} 0.078) and gave the following corrected bond lengths (Å): C1—C2 1.518, C2—C3 1.518, C5—C5^{i} 1.477 Å. The corrections to the other bonds, C2—C4 and C4—C5, were calculated as zero, which is consistent with the expected libration pattern of the molecule.

Data collection: *P*3 (Nicolet, 1987); cell refinement: *P*3; data reduction: *XDISK* (Nicolet, 1987); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

Financial support from the Fonds der Chemischen Industrie is gratefully acknowledged. We thank Mr A. Weinkauf for technical assistance.

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