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1,1,6,6-Tetrakis(4-ethylphenyl)-1,2,3,4,5-hexapentaene

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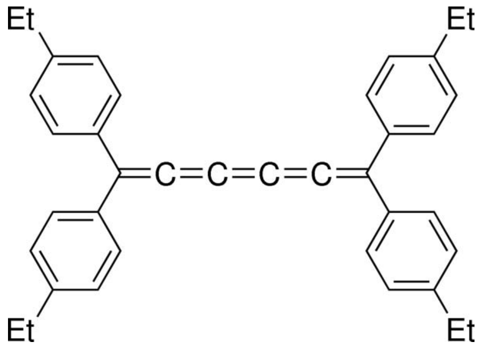
Key indicators: single-crystal X-ray study; T = 90 K; mean σ(C–C) = 0.003 Å; R factor = 0.058; wR factor = 0.166; data-to-parameter ratio = 17.2.

The title compound, (4-$EtC_6H_4)_2C$═C═C═C═C═C(4-$EtC_6H_4)_2$ or $C_{38}H_{36}$, was prepared from 1,1,6,6-tetrakis(4-ethylphenyl)-2,4-hexadiyne-1,6-diol by reduction with $SnCl_2$ in an acidic medium. The molecule has a centre of symmetry at the mid-point of the cumulative double bonds, in which longer and shorter bonds alternate.

Related literature

For related literature, see: Hino *et al.* (2003); Irngartinger & Jäger (1976); Kminek *et al.* (1993); Kuhn & Wallenfels (1938); Kuwatani *et al.* (2005); Woolfson (1953).



Experimental

Crystal data

$C_{38}H_{36}$
M_r = 492.67
Triclinic, $P\overline{1}$
a = 6.233 (3) Å
b = 7.819 (3) Å
c = 15.060 (6) Å
α = 93.849 (7)°
β = 96.353 (6)°
γ = 105.908 (8)°
V = 697.8 (5) $Å^3$
Z = 1
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 90 K
0.20 × 0.08 × 0.03 mm

Data collection

Rigaku AFC-8 diffractometer with Saturn70 CCD detector
Absorption correction: none
10184 measured reflections
3169 independent reflections
2271 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.166
S = 1.10
3169 reflections
184 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.23 e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.349 (2)	C3—$C3^i$	1.310 (3)
C2—C3	1.251 (2)		
C1—C2—C3	177.96 (17)	C2—C3—$C3^i$	177.9 (3)
C2—C1—C4—C9	−21.7 (2)	C2—C1—C12—C13	−39.3 (2)
C2—C1—C4—C5	155.61 (16)	C2—C1—C12—C17	136.72 (17)

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

Data collection: *CrystalClear SM* (Rigaku/MSC, 2005); cell refinement: *CrystalClear SM*; data reduction: *CrystalClear SM*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2187).

References

Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hino, S., Okada, Y., Iwasaki, K., Kijima, M. & Shirakawa, H. (2003). *Chem. Phys. Lett.* **372**, 59–65.
Irngartinger, H. & Jäger, H.-U. (1976). *Angew. Chem. Int. Ed. Engl.* **15**, 562–563.
Kminek, I., Klimovic, J. & Prasad, P. N. (1993). *Chem. Mater.* **5**, 357–360.
Kuhn, R. & Wallenfels, K. (1938). *Ber. Deutsch. Chem. Ges. B*, **71**, 783–790.
Kuwatani, Y., Yamamoto, G., Oda, M. & Iyoda, M. (2005). *Bull. Chem. Soc. Jpn*, **78**, 2188–2208.
Rigaku/MSC (2005). *CrystalClear SM*. Version 1.3.6. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Woolfson, M. M. (1953). *Acta Cryst.* **6**, 838–841.

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supplementary materials

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1,1,6,6-Tetrakis(4-ethylphenyl)-1,2,3,4,5-hexapentaene

N. Suzuki, **D. Hashizume** and **T. Chihara**

Comment

Compounds with highly cumulative unsaturated carbon-carbon bonds are of interest because of their potential application for electronic and optical materials (Kminek *et al.*, 1993; Hino *et al.*, 2003). Hexapentaenes contain six collinear carbon atoms with five cumulative double bonds, and various derivatives have been synthesized (Kuhn & Wallenfels, 1938; Kuwatani *et al.*, 2005). Nevertheless, there have been only two reports on the structural characterization of hexapentaenes. One has 2,2,5,5-tetramethylcyclohexyl groups at the termini of cumulated double bonds (Irngartinger & Jäger, 1976), and atomic coordinates were not provided in the report. The other is 1,1,6,6-tetraphenyl-1,2,3,4,5-hexapentaene reported in 1953 (Woolfson, 1953), which is a pioneering work, although the quality of the analysis does not meet modern standards. Here, we report a novel hexapentaene that has four 4-ethylphenyl groups at the termini of a hexapentaene moiety.

The molecular structure of the title compound, (I), is shown in Fig. 1. The molecule has a symmetry centre, which corresponds to a crystallographic inversion centre, at the middle of six collinear carbon atoms. The longer and shorter bonds alternate in the cumulative double bonds, and C1—C2, C2—C3 and C3—C3^{i} were 1.349 (2), 1.251 (2) and 1.310 (3) Å, respectively, showing a similar tendency to those of reported examples [symmetry code: (i) $1-x, 1-y, 1-z$]. The two benzene rings at the termini were rotated by 22.07 (10)° and 42.01 (7)° from the central mean plane formed by C1—C4, C12, C1^{i}—C4^{i} and C12^{i}. These were rotated in the same direction, whereas it was proposed in 1,1,6,6-tetraphenyl-1,2,3,4,5-hexapentaene (Woolfson, 1953) that corresponding phenyl groups were rotated in opposite direction by 32°. Packing of the molecules is shown in Fig. 2. The molecules of (I) align along the [1 $\bar{1}$ 0] direction so as to make the central mean planes coplanar; the largest deviation between the mean planes of the neighbouring molecules along the direction is 0.037 (9) Å. The coplanes are stacked along the [1 1 0] direction. The distances between the least-square planes of the coplanes, *i.e.* the planes C1—C4/C12/C1^{i}—C4^{i}/C12^{i}/C1^{ii}—C4^{ii}/C12^{ii}/C1^{iii}—C4^{iii}/C12^{iii} and C1^{iv}—C4^{iv}/C12^{iv}/C1^{v}—C4^{v}/C12^{v}/C1^{vi}—C4^{vi}/C12^{vi}/C1^{vii}–C4^{vii}/C12^{vii} [symmetry codes: (ii) $2-x, -y, 1-z$; (iii) $1+x, y-1, z$; (iv) $1+x, y, z$; (v) $2-x, 1-y, 1-z$; (vi) $x, 1+y, z$; (vii) $1-x, 2-y, 1-z$] are 4.12 (2) Å, while in tetraphenylhexapentaene, showing a similar packing motif, the distance between the corresponding planes is *ca* 4 Å.

Experimental

The title compound was prepared according to the reported method (Kuwatani *et al.*, 2005). Hydrogen chloride in diethyl ether (2.0 *M*, 4.76 ml, 9.52 mmol) was added to a solution of 1,1,6,6-tetra(4-ethylphenyl)-2,4-hexadiyne-1,6-diol (1.366 g, 2.38 mmol) and $SnCl_2$ (1.354 g, 7.14 mmol) in THF (15 ml) at 0 °C and stirred for 1 h at 0 °C. Hydrochloric acid (1 N) was added to the dark red solution and extracted with diethyl ether. The organic layer was combined and dried over $MgSO_4$, and volatiles were removed *in vacuo*. The residue was purified by column chromatography on silica gel (hexane/EtOAc = 95/5) to give the title compound as red crystals (yield 0.965 g, 82%; m.p. 125–127 °C). ^{1}H NMR ($CDCl_3$, Me_4Si): δ 1.27 (t, 7.6 Hz, 12H), 2.68 (q, 7.6 Hz, 8H), 7.21 (d, 8.2 Hz, 8H), 7.49 (d, 8.2 Hz, 8H). ^{13}C NMR ($CDCl_3$, Me_4Si): δ 15.46, 28.75, 123.79

(*q*), 126.04 (*q*), 128.03 (CH), 129.34 (CH), 135.76 (q, Ar), 144.87 (q, Ar), 147.84 (*q*). IR (neat, cm^{-1}): 830, 913, 1181, 1457, 1505, 1602, 1656, 1794, 1910, 1999, 2865, 2927, 2964. Calcd for $C_{38}H_{36}$, C 92.64, H 7.36; found C 92.53, H 7.48.

Refinement

All H atoms were found on a difference map and were subsequently treated as riding atoms with C—H distances of 0.95, 0.99 and 0.98 Å for phenyl, methylene and methyl, respectively. The U_{iso}'s of H atoms were fixed to have $1.2U_{eq}$ and $1.5U_{eq}$ of the parent atoms for methylene and phenyl, and methyl, respectively.

Figures

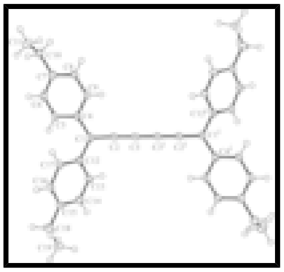


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (i) $1 - x$, $1 - y$, $1 - z$].

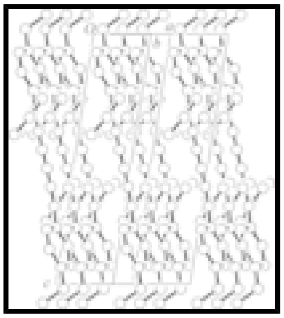


Fig. 2. A packing view of (I).

1,1,6,6-Tetrakis(4-ethylphenyl)-1,2,3,4,5-hexapentaene

Crystal data

$C_{38}H_{36}$	$Z = 1$
$M_r = 492.67$	$F_{000} = 264$
Triclinic, $P\bar{1}$	$D_x = 1.172$ Mg m^{-3}
Hall symbol: -P 1	Mo *K*α radiation λ = 0.71073 Å
$a = 6.233$ (3) Å	Cell parameters from 1421 reflections
$b = 7.819$ (3) Å	θ = 2.7–31.8°
$c = 15.060$ (6) Å	μ = 0.07 mm^{-1}
α = 93.849 (7)°	$T = 90$ K
β = 96.353 (6)°	Plate, red
γ = 105.908 (8)°	0.20 × 0.08 × 0.03 mm
$V = 697.8$ (5) Å^3	

Data collection

Rigaku AFC-8 with Saturn70 CCD detector diffractometer	3169 independent reflections
Radiation source: fine-focus rotating anode	2271 reflections with $I > 2\sigma(I)$
Monochromator: confocal	$R_{\text{int}} = 0.058$
Detector resolution: 28.5714 pixels mm^{-1}	$\theta_{\text{max}} = 27.5°$
$T = 90$ K	$\theta_{\text{min}} = 1.4°$
ω scans	$h = -8 \rightarrow 8$
Absorption correction: none	$k = -10 \rightarrow 10$
10184 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.058$	H-atom parameters constrained
$wR(F^2) = 0.166$	$w = 1/[\sigma^2(F_o^2) + (0.0818P)^2 + 0.1721P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3169 reflections	$\Delta\rho_{\text{max}} = 0.29$ e Å^{-3}
184 parameters	$\Delta\rho_{\text{min}} = -0.22$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.2372 (3)	0.5597 (2)	0.31075 (10)	0.0184 (3)
C2	0.3440 (3)	0.5306 (2)	0.38872 (11)	0.0213 (4)
C3	0.4442 (3)	0.5093 (2)	0.46204 (10)	0.0219 (4)
C4	0.2487 (3)	0.4593 (2)	0.22565 (10)	0.0188 (3)
C5	0.0806 (3)	0.4334 (2)	0.15174 (11)	0.0210 (4)
H5	−0.0388	0.4863	0.1552	0.025*
C6	0.0876 (3)	0.3317 (2)	0.07406 (11)	0.0224 (4)

H7	−0.0276	0.3162	0.0248	0.027*
C7	0.2590 (3)	0.2514 (2)	0.06604 (11)	0.0203 (4)
C8	0.4270 (3)	0.2776 (2)	0.13952 (11)	0.0219 (4)
H8	0.5456	0.2238	0.1358	0.026*
C9	0.4237 (3)	0.3804 (2)	0.21753 (11)	0.0214 (4)
H9	0.5411	0.3979	0.2661	0.026*
C10	0.2656 (3)	0.1413 (2)	−0.01962 (11)	0.0246 (4)
H10A	0.1135	0.1035	−0.0547	0.030*
H10B	0.3064	0.0322	−0.0041	0.030*
C11	0.4330 (3)	0.2429 (3)	−0.07754 (12)	0.0311 (4)
H11A	0.4329	0.1650	−0.1313	0.047*
H11B	0.5840	0.2806	−0.0432	0.047*
H11C	0.3897	0.3483	−0.0953	0.047*
C12	0.1089 (3)	0.6941 (2)	0.31389 (10)	0.0193 (4)
C13	−0.0162 (3)	0.7073 (2)	0.38373 (11)	0.0229 (4)
H13	−0.0273	0.6242	0.4274	0.027*
C14	−0.1250 (3)	0.8395 (2)	0.39083 (12)	0.0251 (4)
H14	−0.2101	0.8450	0.4390	0.030*
C15	−0.1108 (3)	0.9648 (2)	0.32793 (11)	0.0233 (4)
C16	0.0145 (3)	0.9506 (2)	0.25801 (11)	0.0230 (4)
H16	0.0269	1.0345	0.2147	0.028*
C17	0.1212 (3)	0.8180 (2)	0.25001 (11)	0.0215 (4)
H17	0.2033	0.8107	0.2010	0.026*
C18	−0.2284 (4)	1.1101 (3)	0.33273 (14)	0.0367 (5)
H18A	−0.1119	1.2269	0.3447	0.044*
H18B	−0.3142	1.1076	0.2730	0.044*
C19	−0.3871 (3)	1.0999 (3)	0.40214 (13)	0.0320 (4)
H19A	−0.4614	1.1949	0.3965	0.048*
H19B	−0.3022	1.1150	0.4623	0.048*
H19C	−0.5009	0.9833	0.3927	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0181 (7)	0.0202 (8)	0.0174 (8)	0.0065 (6)	−0.0007 (6)	0.0055 (6)
C2	0.0223 (8)	0.0226 (8)	0.0204 (8)	0.0097 (7)	0.0000 (6)	0.0016 (6)
C3	0.0245 (8)	0.0225 (8)	0.0210 (8)	0.0112 (7)	0.0013 (6)	0.0019 (6)
C4	0.0210 (8)	0.0197 (8)	0.0163 (8)	0.0068 (6)	0.0005 (6)	0.0050 (6)
C5	0.0212 (8)	0.0209 (8)	0.0219 (8)	0.0084 (6)	−0.0008 (6)	0.0053 (6)
C6	0.0223 (8)	0.0223 (8)	0.0206 (8)	0.0055 (7)	−0.0049 (6)	0.0040 (6)
C7	0.0226 (8)	0.0173 (8)	0.0193 (8)	0.0023 (6)	0.0026 (6)	0.0042 (6)
C8	0.0229 (8)	0.0240 (8)	0.0223 (8)	0.0115 (7)	0.0030 (6)	0.0059 (6)
C9	0.0215 (8)	0.0250 (8)	0.0179 (8)	0.0081 (7)	−0.0019 (6)	0.0050 (6)
C10	0.0284 (9)	0.0213 (8)	0.0225 (8)	0.0050 (7)	0.0018 (7)	0.0017 (7)
C11	0.0297 (9)	0.0341 (10)	0.0264 (9)	0.0038 (8)	0.0062 (7)	0.0002 (8)
C12	0.0183 (8)	0.0221 (8)	0.0172 (8)	0.0072 (6)	−0.0025 (6)	0.0027 (6)
C13	0.0256 (8)	0.0235 (8)	0.0218 (8)	0.0099 (7)	0.0021 (6)	0.0073 (6)
C14	0.0282 (9)	0.0275 (9)	0.0239 (9)	0.0126 (7)	0.0076 (7)	0.0064 (7)

C15	0.0265 (9)	0.0222 (8)	0.0239 (9)	0.0117 (7)	0.0020 (7)	0.0036 (7)
C16	0.0268 (9)	0.0230 (8)	0.0213 (8)	0.0101 (7)	0.0020 (6)	0.0069 (6)
C17	0.0225 (8)	0.0250 (8)	0.0182 (8)	0.0094 (7)	0.0001 (6)	0.0043 (6)
C18	0.0477 (12)	0.0315 (10)	0.0433 (11)	0.0250 (9)	0.0166 (9)	0.0153 (9)
C19	0.0367 (10)	0.0335 (10)	0.0307 (10)	0.0199 (9)	0.0008 (8)	0.0007 (8)

Geometric parameters (Å, °)

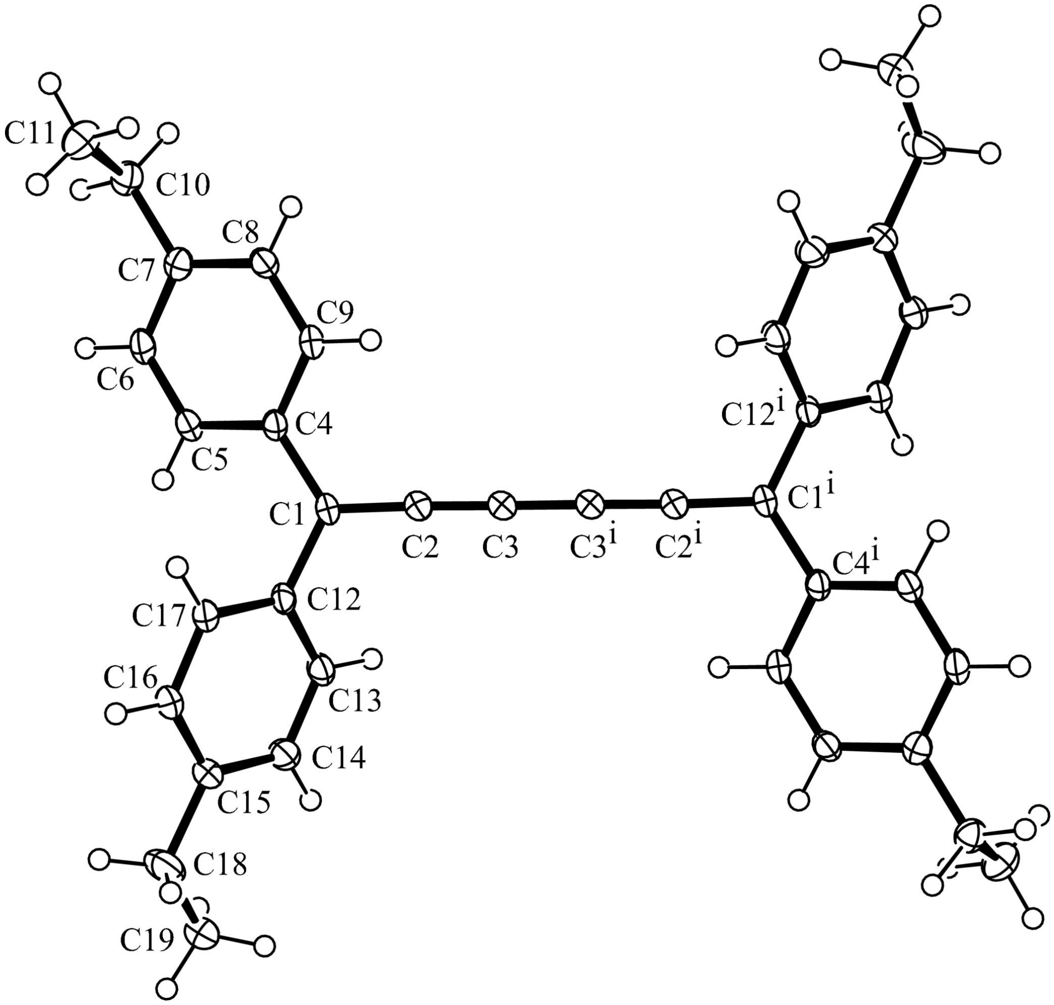
C1—C2	1.349 (2)	C11—H11B	0.9800
C1—C4	1.477 (2)	C11—H11C	0.9800
C1—C12	1.486 (2)	C12—C13	1.391 (2)
C2—C3	1.251 (2)	C12—C17	1.404 (2)
C3—C3$^{\mathrm{i}}$	1.310 (3)	C13—C14	1.387 (2)
C4—C9	1.404 (2)	C13—H13	0.9500
C4—C5	1.405 (2)	C14—C15	1.400 (2)
C5—C6	1.381 (2)	C14—H14	0.9500
C5—H5	0.9500	C15—C16	1.395 (2)
C6—C7	1.392 (2)	C15—C18	1.513 (2)
C6—H7	0.9500	C16—C17	1.382 (2)
C7—C8	1.399 (2)	C16—H16	0.9500
C7—C10	1.513 (2)	C17—H17	0.9500
C8—C9	1.384 (2)	C18—C19	1.508 (3)
C8—H8	0.9500	C18—H18A	0.9900
C9—H9	0.9500	C18—H18B	0.9900
C10—C11	1.523 (2)	C19—H19A	0.9800
C10—H10A	0.9900	C19—H19B	0.9800
C10—H10B	0.9900	C19—H19C	0.9800
C11—H11A	0.9800		
C2—C1—C4	120.27 (14)	H11A—C11—H11C	109.5
C2—C1—C12	117.92 (14)	H11B—C11—H11C	109.5
C4—C1—C12	121.81 (13)	C13—C12—C17	118.07 (15)
C1—C2—C3	177.96 (17)	C13—C12—C1	120.59 (14)
C2—C3—C3$^{\mathrm{i}}$	177.9 (3)	C17—C12—C1	121.22 (15)
C9—C4—C5	118.00 (14)	C14—C13—C12	121.30 (15)
C9—C4—C1	120.79 (13)	C14—C13—H13	119.3
C5—C4—C1	121.15 (14)	C12—C13—H13	119.3
C6—C5—C4	120.54 (15)	C13—C14—C15	120.82 (16)
C6—C5—H5	119.7	C13—C14—H14	119.6
C4—C5—H5	119.7	C15—C14—H14	119.6
C5—C6—C7	121.71 (14)	C16—C15—C14	117.61 (15)
C5—C6—H7	119.1	C16—C15—C18	119.85 (15)
C7—C6—H7	119.1	C14—C15—C18	122.53 (16)
C6—C7—C8	117.80 (14)	C17—C16—C15	121.84 (15)
C6—C7—C10	121.20 (14)	C17—C16—H16	119.1
C8—C7—C10	121.00 (15)	C15—C16—H16	119.1
C9—C8—C7	121.23 (15)	C16—C17—C12	120.34 (15)
C9—C8—H8	119.4	C16—C17—H17	119.8
C7—C8—H8	119.4	C12—C17—H17	119.8

C8—C9—C4	120.71 (14)	C19—C18—C15	116.43 (16)
C8—C9—H9	119.6	C19—C18—H18A	108.2
C4—C9—H9	119.6	C15—C18—H18A	108.2
C7—C10—C11	112.81 (14)	C19—C18—H18B	108.2
C7—C10—H10A	109.0	C15—C18—H18B	108.2
C11—C10—H10A	109.0	H18A—C18—H18B	107.3
C7—C10—H10B	109.0	C18—C19—H19A	109.5
C11—C10—H10B	109.0	C18—C19—H19B	109.5
H10A—C10—H10B	107.8	H19A—C19—H19B	109.5
C10—C11—H11A	109.5	C18—C19—H19C	109.5
C10—C11—H11B	109.5	H19A—C19—H19C	109.5
H11A—C11—H11B	109.5	H19B—C19—H19C	109.5
C10—C11—H11C	109.5		

C2—C1—C4—C9	−21.7 (2)	C2—C1—C12—C13	−39.3 (2)
C12—C1—C4—C9	158.52 (15)	C4—C1—C12—C13	140.43 (16)
C2—C1—C4—C5	155.61 (16)	C2—C1—C12—C17	136.72 (17)
C12—C1—C4—C5	−24.1 (2)	C4—C1—C12—C17	−43.5 (2)
C9—C4—C5—C6	0.7 (2)	C17—C12—C13—C14	−0.4 (2)
C1—C4—C5—C6	−176.76 (15)	C1—C12—C13—C14	175.78 (14)
C4—C5—C6—C7	0.2 (3)	C12—C13—C14—C15	−0.4 (3)
C5—C6—C7—C8	−0.4 (2)	C13—C14—C15—C16	0.5 (3)
C5—C6—C7—C10	−179.58 (15)	C13—C14—C15—C18	179.49 (17)
C6—C7—C8—C9	−0.2 (2)	C14—C15—C16—C17	0.2 (2)
C10—C7—C8—C9	178.97 (15)	C18—C15—C16—C17	−178.78 (16)
C7—C8—C9—C4	1.1 (3)	C15—C16—C17—C12	−1.1 (2)
C5—C4—C9—C8	−1.3 (2)	C13—C12—C17—C16	1.1 (2)
C1—C4—C9—C8	176.17 (15)	C1—C12—C17—C16	−175.03 (14)
C6—C7—C10—C11	101.36 (19)	C16—C15—C18—C19	171.39 (16)
C8—C7—C10—C11	−77.8 (2)	C14—C15—C18—C19	−7.6 (3)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1


C11
C10
C8
C7
C9
C6
C4
C5
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C2
C3
$C3^i$
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$C1^i$
$C12^i$
$C4^i$
C12
C17
C16
C13
C14
C15
C18
C19

Fig. 2