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trans-1,2-Difluoro-3,4,5,6,7,8-hexaphenyltricyclo[4.2.0.0^{2,5}]octa-3,7-diene

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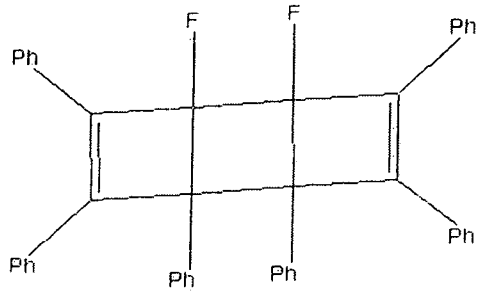
Key indicators: single-crystal X-ray study; T = 400 K; mean σ(C–C) = 0.009 Å; R factor = 0.076; wR factor = 0.241; data-to-parameter ratio = 13.3.

In order to probe the possible mechanism of the rearrangement of *trans*-hexaphenyldifluorotricyclooctadiene (a dimer of fluorotriphenylcyclobutadiene) to pentaphenyldihydrodifluoropentalene *via* C—F bond migration, a high-temperature study of the title compound, $C_{44}H_{30}F_2$, was performed at 400 (2) K. In the title compound, there are three fused four-membered rings with the resulting eight-membered tricyclooctadiene ring adopting a sofa conformation. The dihedral angles between the central four-membered ring and the two outer rings are 66.03 (2) and 65.39 (2)°. The crystal structure contains centrosymmetric dimers formed by C—H$\cdots\pi$ interactions.

Related literature

For background on chemistry of octadienes and their precursors, see: Choudhury *et al.* (2007); Fritchie & Hughes (1962). For the preparation of the title compound, see: Nagarajan *et al.* (1964).



Experimental

Crystal data

$C_{44}H_{30}F_2$
M_r = 596.68
Triclinic, $P\overline{1}$
a = 9.331 (9) Å
b = 13.136 (8) Å
c = 13.614 (9) Å
α = 95.63 (4)°
β = 103.87 (5)°
γ = 91.64 (4)°
V = 1610 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 400 (2) K
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.939, T_{max} = 0.985
11153 measured reflections
5532 independent reflections
3395 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.241
S = 1.10
5532 reflections
415 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C9–C14 ring.

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
C17—H17$\cdots$*Cg*1^{i}	0.93	2.91	3.689 (10)	142

Symmetry code: (i) $-x+2, -y, -z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

We thank the Department of Science and Technology, India, for data collection on the CCD facility set up under the IRHPA–DST program. DC thanks the Indian Institute of Science for a fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2394).

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supplementary materials

Acta Cryst. (2007). E63, o4557 [doi:10.1107/S1600536807054281]

trans-1,2-Difluoro-3,4,5,6,7,8-hexaphenyltricyclo[4.2.0.0^{2,5}]octa-3,7-diene

D. Chopra, K. Nagarajan, J. D. Roberts and T. N. Guru Row

Comment

The chemistry of fluorotriphenylcyclobutadiene, a monomer of the title compound is well known (Fritchie & Hughes, 1962). In order to investigate and probe the possible mechanism of rearrangement of *trans*-hexaphenyldifluorotricyclooctadiene, (a dimer of fluorotriphenylcyclobutadiene), to pentaphenyldihydrodifluoropentalene *via* C—F bond migration (Choudhury *et al.*,2007), a high temperature study of the title compound was performed at 400 (2) K. It was hoped that at that temperature C—F bond cleavage would occur to produce the rearrangement product pentaphenyldihydrodifluoropentalene. However, no additional migratory process was in fact observed.

The eight-membered cyclooctadiene ring exists in a sofa conformation, Fig 1. This also depicts the relative disposition of the phenyl and fluoro substituents around the eight-membered ring. The dihedral angles between the central four membered ring and the two fused four membered rings other rings on either side are 66.03 (2)° and 65.39 (2)° respectively. The crystal structure is stabilized by the formation of inversion related dimers linked by C—H···π interactions (Fig. 2).

Experimental

The title compound was synthesized in accordance with the procedure reported in literature (Nagarajan *et al.*, 1964). Crystals were obtained by recrystallization from chloroform and ethanol 2:1 (v:v).

Refinement

All the H atoms were fixed in calculated positions and allowed to ride on the parent carbon atoms with C—H = 0.93Å and $U_{(eq)}H = 1.2\ U_{(eq)}C$.

Figures

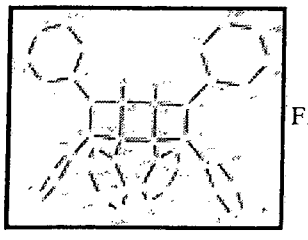

Fig. 1. The structure of (I) with displacement ellipsoids drawn at the 10% probability level.

Fig. 2. Partial packing diagram for (I). The dotted lines show the C—H···π interactions.

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Crystal data

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$M_r = 596.68$

Triclinic, $P\overline{1}$

Hall symbol: -P 1

$a = 9.331\ (9)$ Å

$b = 13.136\ (8)$ Å

$c = 13.614\ (9)$ Å

$\alpha = 95.63\ (4)°$

$\beta = 103.87\ (5)°$

$\gamma = 91.64\ (4)°$

$V = 1610\ (2)$ Å^3

$Z = 2$

$F_{000} = 624$

$D_x = 1.231$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 963 reflections

$\theta = 1.2–25.8°$

$\mu = 0.08$ mm^{-1}

$T = 400\ (2)$ K

Block, yellow

0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 400(2)$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1997)

$T_{min} = 0.939$, $T_{max} = 0.985$

11153 measured reflections

5532 independent reflections

3395 reflections with $I > 2\sigma(I)$

$R_{int} = 0.033$

$\theta_{max} = 25.0°$

$\theta_{min} = 2.1°$

$h = -11 \rightarrow 11$

$k = -15 \rightarrow 14$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.076$

$wR(F^2) = 0.241$

$S = 1.10$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1465P)^2 + 1.8307P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = <0.001$

5532 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
415 parameters	$\Delta\rho_{min} = -0.18$ 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 $F^2 > 2\text{sigma}(F^2)$ 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}
F1	0.0988 (3)	0.5834 (2)	0.7694 (2)	0.0832 (9)
F2	0.3326 (3)	0.7528 (2)	0.9294 (2)	0.0816 (8)
C1	0.0157 (5)	0.7480 (4)	0.8309 (4)	0.0670 (12)
C2	0.1247 (5)	0.6883 (3)	0.7876 (3)	0.0630 (11)
C3	0.2854 (5)	0.7249 (3)	0.8255 (3)	0.0644 (11)
C4	0.3944 (5)	0.6710 (3)	0.7758 (4)	0.0660 (12)
C5	0.3756 (5)	0.7329 (3)	0.7007 (4)	0.0649 (12)
C6	0.2698 (5)	0.8024 (3)	0.7434 (3)	0.0614 (11)
C7	0.1033 (5)	0.7629 (3)	0.7015 (3)	0.0632 (11)
C8	0.0040 (5)	0.8169 (3)	0.7631 (4)	0.0650 (12)
C9	−0.0453 (5)	0.7314 (4)	0.9179 (4)	0.0670 (12)
C10	0.0107 (6)	0.6607 (4)	0.9826 (4)	0.0831 (15)
C11	−0.0489 (7)	0.6420 (5)	1.0628 (5)	0.1032 (19)
C12	−0.1666 (8)	0.6948 (6)	1.0779 (6)	0.114 (2)
C13	−0.2266 (8)	0.7630 (6)	1.0125 (6)	0.116 (2)
C14	−0.1683 (6)	0.7814 (5)	0.9334 (5)	0.0927 (17)
C15	−0.0660 (5)	0.9150 (4)	0.7530 (4)	0.0716 (13)
C16	−0.0491 (7)	0.9888 (4)	0.8345 (5)	0.0972 (18)
C17	−0.1156 (9)	1.0801 (5)	0.8242 (7)	0.119 (2)
C18	−0.1996 (9)	1.0989 (6)	0.7330 (9)	0.128 (3)
C19	−0.2165 (8)	1.0285 (6)	0.6499 (7)	0.119 (2)
C20	−0.1501 (7)	0.9369 (5)	0.6589 (5)	0.0970 (18)
C21	0.0383 (5)	0.7255 (4)	0.5918 (4)	0.0696 (12)
C22	−0.0656 (8)	0.6452 (5)	0.5655 (5)	0.112 (2)
C23	−0.1263 (11)	0.6109 (6)	0.4661 (7)	0.143 (3)
C24	−0.0855 (11)	0.6533 (7)	0.3888 (6)	0.131 (3)
C25	0.0112 (9)	0.7332 (7)	0.4122 (5)	0.124 (2)
C26	0.0749 (7)	0.7683 (5)	0.5136 (5)	0.0997 (18)

C27	0.3174 (6)	0.9143 (3)	0.7669 (4)	0.0673 (12)
C28	0.2478 (7)	0.9871 (4)	0.7095 (5)	0.0904 (17)
C29	0.3028 (9)	1.0887 (5)	0.7281 (7)	0.112 (2)
C30	0.4252 (11)	1.1161 (5)	0.8035 (8)	0.119 (3)
C31	0.4954 (9)	1.0448 (6)	0.8624 (6)	0.113 (2)
C32	0.4416 (7)	0.9445 (5)	0.8426 (5)	0.0894 (16)
C33	0.4231 (5)	0.7315 (4)	0.6055 (4)	0.0689 (12)
C34	0.4755 (6)	0.8186 (5)	0.5754 (4)	0.0848 (15)
C35	0.5170 (7)	0.8162 (6)	0.4848 (5)	0.1024 (19)
C36	0.5067 (9)	0.7271 (7)	0.4249 (6)	0.121 (2)
C37	0.4569 (11)	0.6399 (6)	0.4538 (6)	0.133 (3)
C38	0.4153 (8)	0.6422 (5)	0.5436 (5)	0.105 (2)
C39	0.4800 (6)	0.5821 (4)	0.8010 (4)	0.0725 (13)
C40	0.6126 (6)	0.5707 (5)	0.7734 (5)	0.0930 (17)
C41	0.6933 (8)	0.4874 (6)	0.7985 (6)	0.111 (2)
C42	0.6456 (9)	0.4145 (5)	0.8489 (6)	0.114 (2)
C43	0.5171 (8)	0.4254 (5)	0.8790 (6)	0.110 (2)
C44	0.4351 (7)	0.5089 (4)	0.8551 (5)	0.0928 (17)
H10	0.0909	0.6244	0.9721	0.100*
H11	−0.0092	0.5939	1.1061	0.124*
H12	−0.2060	0.6844	1.1330	0.137*
H13	−0.3087	0.7974	1.0222	0.140*
H14	−0.2111	0.8279	0.8892	0.111*
H16	0.0084	0.9766	0.8977	0.117*
H17	−0.1029	1.1292	0.8801	0.142*
H18	−0.2463	1.1604	0.7268	0.154*
H19	−0.2731	1.0426	0.5870	0.143*
H20	−0.1612	0.8893	0.6021	0.116*
H22	−0.0951	0.6137	0.6163	0.135*
H23	−0.1976	0.5570	0.4505	0.171*
H24	−0.1245	0.6268	0.3214	0.157*
H25	0.0365	0.7659	0.3607	0.148*
H26	0.1450	0.8230	0.5284	0.120*
H28	0.1633	0.9685	0.6579	0.109*
H29	0.2554	1.1376	0.6888	0.134*
H30	0.4621	1.1839	0.8155	0.143*
H31	0.5784	1.0640	0.9150	0.135*
H32	0.4907	0.8959	0.8815	0.107*
H34	0.4832	0.8802	0.6167	0.102*
H35	0.5521	0.8760	0.4650	0.123*
H36	0.5338	0.7256	0.3633	0.145*
H37	0.4511	0.5783	0.4127	0.160*
H38	0.3812	0.5819	0.5629	0.126*
H40	0.6468	0.6193	0.7379	0.112*
H41	0.7829	0.4808	0.7805	0.133*
H42	0.7003	0.3573	0.8629	0.137*
H44	0.3476	0.5162	0.8758	0.111*
H43	0.4851	0.3768	0.9154	0.132*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.095 (2)	0.0582 (16)	0.100 (2)	0.0018 (14)	0.0290 (17)	0.0104 (14)
F2	0.0918 (19)	0.0848 (19)	0.0679 (18)	0.0097 (15)	0.0171 (15)	0.0111 (14)
C1	0.066 (3)	0.068 (3)	0.069 (3)	0.007 (2)	0.018 (2)	0.009 (2)
C2	0.073 (3)	0.053 (2)	0.066 (3)	0.009 (2)	0.021 (2)	0.012 (2)
C3	0.076 (3)	0.062 (3)	0.056 (3)	0.009 (2)	0.016 (2)	0.007 (2)
C4	0.070 (3)	0.059 (3)	0.071 (3)	0.008 (2)	0.019 (2)	0.009 (2)
C5	0.068 (3)	0.054 (2)	0.072 (3)	0.000 (2)	0.019 (2)	0.001 (2)
C6	0.069 (3)	0.056 (2)	0.062 (3)	0.007 (2)	0.021 (2)	0.008 (2)
C7	0.070 (3)	0.056 (3)	0.066 (3)	0.008 (2)	0.021 (2)	0.007 (2)
C8	0.067 (3)	0.060 (3)	0.070 (3)	0.007 (2)	0.019 (2)	0.007 (2)
C9	0.069 (3)	0.067 (3)	0.067 (3)	0.007 (2)	0.019 (2)	0.012 (2)
C10	0.081 (3)	0.089 (4)	0.088 (4)	0.014 (3)	0.030 (3)	0.021 (3)
C11	0.102 (5)	0.119 (5)	0.097 (4)	0.008 (4)	0.028 (4)	0.043 (4)
C12	0.097 (5)	0.159 (7)	0.103 (5)	0.011 (4)	0.048 (4)	0.037 (5)
C13	0.096 (4)	0.157 (6)	0.120 (5)	0.033 (4)	0.058 (4)	0.042 (5)
C14	0.083 (4)	0.117 (5)	0.091 (4)	0.027 (3)	0.034 (3)	0.033 (3)
C15	0.066 (3)	0.066 (3)	0.089 (4)	0.009 (2)	0.026 (3)	0.014 (3)
C16	0.104 (4)	0.081 (4)	0.108 (5)	0.013 (3)	0.030 (4)	0.003 (3)
C17	0.122 (6)	0.077 (4)	0.163 (8)	0.018 (4)	0.053 (6)	−0.005 (4)
C18	0.106 (5)	0.080 (5)	0.212 (10)	0.031 (4)	0.052 (6)	0.041 (6)
C19	0.107 (5)	0.102 (5)	0.146 (7)	0.034 (4)	0.014 (5)	0.042 (5)
C20	0.089 (4)	0.089 (4)	0.109 (5)	0.019 (3)	0.009 (3)	0.028 (3)
C21	0.069 (3)	0.066 (3)	0.072 (3)	0.006 (2)	0.014 (2)	0.011 (2)
C22	0.133 (6)	0.104 (5)	0.086 (4)	−0.037 (4)	0.005 (4)	0.011 (4)
C23	0.171 (8)	0.114 (6)	0.111 (6)	−0.045 (5)	−0.015 (6)	−0.002 (5)
C24	0.155 (7)	0.136 (7)	0.085 (5)	−0.002 (6)	0.004 (5)	−0.003 (5)
C25	0.128 (6)	0.168 (8)	0.073 (4)	−0.006 (6)	0.018 (4)	0.023 (5)
C26	0.096 (4)	0.114 (5)	0.083 (4)	−0.012 (4)	0.009 (3)	0.024 (4)
C27	0.075 (3)	0.058 (3)	0.075 (3)	0.006 (2)	0.032 (3)	0.004 (2)
C28	0.088 (4)	0.067 (3)	0.128 (5)	0.014 (3)	0.042 (3)	0.028 (3)
C29	0.125 (6)	0.067 (4)	0.169 (7)	0.015 (4)	0.080 (6)	0.027 (4)
C30	0.140 (7)	0.071 (4)	0.160 (7)	−0.024 (4)	0.079 (6)	−0.017 (5)
C31	0.126 (6)	0.096 (5)	0.114 (5)	−0.031 (4)	0.042 (4)	−0.020 (4)
C32	0.097 (4)	0.084 (4)	0.085 (4)	−0.013 (3)	0.025 (3)	−0.004 (3)
C33	0.068 (3)	0.069 (3)	0.072 (3)	0.009 (2)	0.021 (2)	0.009 (2)
C34	0.092 (4)	0.089 (4)	0.080 (4)	0.004 (3)	0.032 (3)	0.013 (3)
C35	0.112 (5)	0.112 (5)	0.099 (5)	0.014 (4)	0.047 (4)	0.033 (4)
C36	0.148 (6)	0.144 (7)	0.084 (5)	0.042 (5)	0.047 (4)	0.021 (5)
C37	0.206 (9)	0.104 (5)	0.099 (5)	0.020 (5)	0.061 (6)	−0.015 (4)
C38	0.159 (6)	0.076 (4)	0.084 (4)	0.003 (4)	0.043 (4)	−0.006 (3)
C39	0.075 (3)	0.060 (3)	0.079 (3)	0.012 (2)	0.012 (3)	0.003 (2)
C40	0.084 (4)	0.091 (4)	0.105 (4)	0.022 (3)	0.024 (3)	0.012 (3)
C41	0.090 (4)	0.111 (5)	0.129 (6)	0.039 (4)	0.019 (4)	0.003 (4)
C42	0.104 (5)	0.080 (4)	0.140 (6)	0.033 (4)	−0.009 (4)	0.008 (4)

C43	0.112 (5)	0.078 (4)	0.133 (6)	0.016 (4)	0.006 (4)	0.032 (4)
C44	0.093 (4)	0.076 (4)	0.114 (5)	0.019 (3)	0.026 (3)	0.027 (3)

Geometric parameters (Å, °)

F1—C2	1.381 (5)	C20—C19	1.372 (9)
F2—C3	1.385 (5)	C20—H20	0.9300
C8—C1	1.344 (6)	C44—C43	1.376 (8)
C8—C15	1.465 (6)	C44—H44	0.9300
C8—C7	1.536 (6)	C35—C36	1.346 (10)
C7—C21	1.498 (7)	C35—H35	0.9300
C7—C6	1.574 (7)	C30—C29	1.353 (11)
C7—C2	1.581 (6)	C30—C31	1.371 (11)
C6—C27	1.504 (7)	C30—H30	0.9300
C6—C5	1.539 (6)	C22—C23	1.361 (10)
C6—C3	1.570 (6)	C22—H22	0.9300
C5—C4	1.350 (6)	C42—C41	1.356 (10)
C5—C33	1.466 (7)	C42—C43	1.364 (10)
C9—C10	1.372 (7)	C42—H42	0.9300
C9—C14	1.387 (7)	C40—C41	1.370 (8)
C9—C1	1.462 (7)	C40—H40	0.9300
C4—C39	1.456 (6)	C29—H29	0.9300
C4—C3	1.506 (6)	C38—C37	1.366 (9)
C3—C2	1.511 (7)	C38—H38	0.9300
C2—C1	1.497 (6)	C41—H41	0.9300
C33—C38	1.366 (7)	C11—C12	1.362 (9)
C33—C34	1.368 (7)	C11—H11	0.9300
C39—C44	1.380 (8)	C18—C17	1.349 (11)
C39—C40	1.386 (8)	C18—C19	1.365 (12)
C21—C26	1.359 (8)	C18—H18	0.9300
C21—C22	1.372 (8)	C17—H17	0.9300
C27—C28	1.374 (7)	C37—C36	1.353 (11)
C27—C32	1.372 (8)	C37—H37	0.9300
C15—C16	1.376 (8)	C26—C25	1.393 (9)
C15—C20	1.394 (8)	C26—H26	0.9300
C34—C35	1.377 (8)	C43—H43	0.9300
C34—H34	0.9300	C31—H31	0.9300
C32—C31	1.373 (9)	C12—C13	1.362 (9)
C32—H32	0.9300	C12—H12	0.9300
C28—C29	1.393 (9)	C13—H13	0.9300
C28—H28	0.9300	C36—H36	0.9300
C10—C11	1.377 (8)	C19—H19	0.9300
C10—H10	0.9300	C25—C24	1.328 (11)
C14—C13	1.356 (8)	C25—H25	0.9300
C14—H14	0.9300	C24—C23	1.362 (11)
C16—C17	1.370 (9)	C24—H24	0.9300
C16—H16	0.9300	C23—H23	0.9300
C1—C8—C15	133.9 (4)	C19—C20—C15	120.3 (7)
C1—C8—C7	95.5 (4)	C19—C20—H20	119.9

C15—C8—C7	130.3 (4)	C15—C20—H20	119.9
C21—C7—C8	118.7 (4)	C43—C44—C39	121.4 (6)
C21—C7—C6	122.8 (4)	C43—C44—H44	119.3
C8—C7—C6	111.3 (4)	C39—C44—H44	119.3
C21—C7—C2	121.8 (4)	C36—C35—C34	119.8 (7)
C8—C7—C2	83.1 (3)	C36—C35—H35	120.1
C6—C7—C2	89.0 (3)	C34—C35—H35	120.1
C27—C6—C5	116.2 (4)	C29—C30—C31	120.5 (7)
C27—C6—C3	124.2 (4)	C29—C30—H30	119.7
C5—C6—C3	83.9 (3)	C31—C30—H30	119.7
C27—C6—C7	122.9 (4)	C23—C22—C21	120.9 (7)
C5—C6—C7	112.2 (4)	C23—C22—H22	119.6
C3—C6—C7	88.7 (3)	C21—C22—H22	119.6
C4—C5—C33	134.2 (4)	C41—C42—C43	119.7 (6)
C4—C5—C6	94.9 (4)	C41—C42—H42	120.2
C33—C5—C6	130.7 (4)	C43—C42—H42	120.2
C10—C9—C14	117.8 (5)	C41—C40—C39	119.7 (6)
C10—C9—C1	121.1 (4)	C41—C40—H40	120.2
C14—C9—C1	121.0 (5)	C39—C40—H40	120.2
C5—C4—C39	135.4 (5)	C30—C29—C28	119.9 (7)
C5—C4—C3	93.2 (4)	C30—C29—H29	120.1
C39—C4—C3	131.3 (4)	C28—C29—H29	120.1
F2—C3—C4	116.2 (4)	C37—C38—C33	121.1 (6)
F2—C3—C2	115.4 (4)	C37—C38—H38	119.4
C4—C3—C2	117.1 (4)	C33—C38—H38	119.4
F2—C3—C6	124.0 (4)	C42—C41—C40	121.6 (7)
C4—C3—C6	87.7 (3)	C42—C41—H41	119.2
C2—C3—C6	91.7 (3)	C40—C41—H41	119.2
F1—C2—C1	117.1 (4)	C12—C11—C10	119.2 (6)
F1—C2—C3	115.2 (4)	C12—C11—H11	120.4
C1—C2—C3	116.7 (4)	C10—C11—H11	120.4
F1—C2—C7	124.3 (4)	C17—C18—C19	120.5 (7)
C1—C2—C7	87.9 (3)	C17—C18—H18	119.7
C3—C2—C7	90.5 (3)	C19—C18—H18	119.7
C38—C33—C34	117.9 (5)	C18—C17—C16	120.1 (7)
C38—C33—C5	120.4 (5)	C18—C17—H17	120.0
C34—C33—C5	121.7 (5)	C16—C17—H17	120.0
C44—C39—C40	118.1 (5)	C36—C37—C38	120.0 (7)
C44—C39—C4	121.8 (5)	C36—C37—H37	120.0
C40—C39—C4	120.1 (5)	C38—C37—H37	120.0
C26—C21—C22	116.3 (5)	C21—C26—C25	122.3 (6)
C26—C21—C7	123.3 (5)	C21—C26—H26	118.9
C22—C21—C7	120.4 (5)	C25—C26—H26	118.9
C28—C27—C32	118.2 (5)	C42—C43—C44	119.5 (7)
C28—C27—C6	122.1 (5)	C42—C43—H43	120.2
C32—C27—C6	119.5 (5)	C44—C43—H43	120.2
C8—C1—C9	136.9 (4)	C30—C31—C32	119.2 (7)
C8—C1—C2	93.2 (4)	C30—C31—H31	120.4
C9—C1—C2	129.9 (4)	C32—C31—H31	120.4

C16—C15—C20	117.9 (5)	C11—C12—C13	120.0 (6)
C16—C15—C8	121.7 (5)	C11—C12—H12	120.0
C20—C15—C8	120.4 (5)	C13—C12—H12	120.0
C33—C34—C35	120.9 (6)	C14—C13—C12	120.9 (6)
C33—C34—H34	119.6	C14—C13—H13	119.5
C35—C34—H34	119.6	C12—C13—H13	119.5
C31—C32—C27	121.7 (7)	C35—C36—C37	120.2 (7)
C31—C32—H32	119.1	C35—C36—H36	119.9
C27—C32—H32	119.1	C37—C36—H36	119.9
C27—C28—C29	120.5 (7)	C18—C19—C20	120.0 (7)
C27—C28—H28	119.8	C18—C19—H19	120.0
C29—C28—H28	119.8	C20—C19—H19	120.0
C9—C10—C11	121.6 (5)	C24—C25—C26	120.2 (7)
C9—C10—H10	119.2	C24—C25—H25	119.9
C11—C10—H10	119.2	C26—C25—H25	119.9
C13—C14—C9	120.5 (6)	C25—C24—C23	118.3 (7)
C13—C14—H14	119.8	C25—C24—H24	120.9
C9—C14—H14	119.8	C23—C24—H24	120.9
C17—C16—C15	121.1 (7)	C22—C23—C24	121.9 (8)
C17—C16—H16	119.5	C22—C23—H23	119.0
C15—C16—H16	119.5	C24—C23—H23	119.0
C1—C8—C7—C21	118.4 (4)	C5—C6—C27—C28	109.3 (5)
C15—C8—C7—C21	−66.3 (7)	C3—C6—C27—C28	−149.7 (5)
C1—C8—C7—C6	−90.5 (4)	C7—C6—C27—C28	−35.8 (7)
C15—C8—C7—C6	84.9 (6)	C5—C6—C27—C32	−65.1 (6)
C1—C8—C7—C2	−4.2 (4)	C3—C6—C27—C32	35.9 (6)
C15—C8—C7—C2	171.1 (5)	C7—C6—C27—C32	149.8 (5)
C21—C7—C6—C27	102.4 (5)	C15—C8—C1—C9	7.9 (10)
C8—C7—C6—C27	−47.4 (6)	C7—C8—C1—C9	−177.0 (6)
C2—C7—C6—C27	−129.6 (4)	C15—C8—C1—C2	−170.6 (5)
C21—C7—C6—C5	−43.9 (6)	C7—C8—C1—C2	4.4 (4)
C8—C7—C6—C5	166.4 (4)	C10—C9—C1—C8	−168.7 (6)
C2—C7—C6—C5	84.2 (4)	C14—C9—C1—C8	15.9 (9)
C21—C7—C6—C3	−126.8 (4)	C10—C9—C1—C2	9.4 (8)
C8—C7—C6—C3	83.5 (4)	C14—C9—C1—C2	−166.0 (5)
C2—C7—C6—C3	1.3 (3)	F1—C2—C1—C8	−132.2 (4)
C27—C6—C5—C4	121.7 (4)	C3—C2—C1—C8	85.2 (5)
C3—C6—C5—C4	−3.5 (4)	C7—C2—C1—C8	−4.3 (4)
C7—C6—C5—C4	−89.6 (4)	F1—C2—C1—C9	49.1 (7)
C27—C6—C5—C33	−63.9 (7)	C3—C2—C1—C9	−93.5 (6)
C3—C6—C5—C33	170.8 (5)	C7—C2—C1—C9	177.0 (5)
C7—C6—C5—C33	84.8 (6)	C1—C8—C15—C16	46.0 (8)
C33—C5—C4—C39	7.1 (10)	C7—C8—C15—C16	−127.5 (6)
C6—C5—C4—C39	−178.8 (6)	C1—C8—C15—C20	−135.2 (6)
C33—C5—C4—C3	−170.4 (5)	C7—C8—C15—C20	51.2 (7)
C6—C5—C4—C3	3.7 (4)	C38—C33—C34—C35	0.9 (9)
C5—C4—C3—F2	−130.8 (4)	C5—C33—C34—C35	−178.8 (5)
C39—C4—C3—F2	51.5 (7)	C28—C27—C32—C31	0.9 (8)
C5—C4—C3—C2	87.2 (5)	C6—C27—C32—C31	175.5 (5)

C39—C4—C3—C2	−90.5 (6)	C32—C27—C28—C29	0.1 (8)
C5—C4—C3—C6	−3.6 (4)	C6—C27—C28—C29	−174.4 (5)
C39—C4—C3—C6	178.7 (5)	C14—C9—C10—C11	−2.4 (9)
C27—C6—C3—F2	6.0 (7)	C1—C9—C10—C11	−177.9 (5)
C5—C6—C3—F2	123.6 (5)	C10—C9—C14—C13	2.4 (9)
C7—C6—C3—F2	−123.9 (4)	C1—C9—C14—C13	178.0 (6)
C27—C6—C3—C4	−114.5 (5)	C20—C15—C16—C17	1.5 (9)
C5—C6—C3—C4	3.2 (3)	C8—C15—C16—C17	−179.8 (6)
C7—C6—C3—C4	115.7 (3)	C16—C15—C20—C19	−1.8 (9)
C27—C6—C3—C2	128.5 (4)	C8—C15—C20—C19	179.5 (6)
C5—C6—C3—C2	−113.9 (3)	C40—C39—C44—C43	−1.6 (9)
C7—C6—C3—C2	−1.3 (3)	C4—C39—C44—C43	−179.7 (6)
F2—C3—C2—F1	−100.5 (4)	C33—C34—C35—C36	−0.3 (10)
C4—C3—C2—F1	41.8 (6)	C26—C21—C22—C23	0.6 (10)
C6—C3—C2—F1	130.2 (4)	C7—C21—C22—C23	179.6 (7)
F2—C3—C2—C1	42.8 (5)	C44—C39—C40—C41	1.1 (9)
C4—C3—C2—C1	−174.9 (4)	C4—C39—C40—C41	179.2 (5)
C6—C3—C2—C1	−86.5 (4)	C31—C30—C29—C28	−0.4 (11)
F2—C3—C2—C7	130.7 (4)	C27—C28—C29—C30	−0.3 (9)
C4—C3—C2—C7	−87.0 (4)	C34—C33—C38—C37	−0.8 (10)
C6—C3—C2—C7	1.3 (3)	C5—C33—C38—C37	179.0 (7)
C21—C7—C2—F1	6.0 (6)	C43—C42—C41—C40	−2.5 (11)
C8—C7—C2—F1	125.6 (4)	C39—C40—C41—C42	0.9 (10)
C6—C7—C2—F1	−122.8 (4)	C9—C10—C11—C12	0.2 (10)
C21—C7—C2—C1	−115.8 (4)	C19—C18—C17—C16	−1.5 (12)
C8—C7—C2—C1	3.8 (3)	C15—C16—C17—C18	0.1 (11)
C6—C7—C2—C1	115.4 (3)	C33—C38—C37—C36	−0.1 (13)
C21—C7—C2—C3	127.5 (4)	C22—C21—C26—C25	0.0 (10)
C8—C7—C2—C3	−112.9 (3)	C7—C21—C26—C25	−179.0 (6)
C6—C7—C2—C3	−1.3 (3)	C41—C42—C43—C44	1.9 (11)
C4—C5—C33—C38	42.7 (9)	C39—C44—C43—C42	0.1 (10)
C6—C5—C33—C38	−129.5 (6)	C29—C30—C31—C32	1.3 (11)
C4—C5—C33—C34	−137.6 (6)	C27—C32—C31—C30	−1.6 (10)
C6—C5—C33—C34	50.2 (8)	C10—C11—C12—C13	1.9 (11)
C5—C4—C39—C44	−152.2 (6)	C9—C14—C13—C12	−0.4 (11)
C3—C4—C39—C44	24.5 (8)	C11—C12—C13—C14	−1.8 (12)
C5—C4—C39—C40	29.7 (9)	C34—C35—C36—C37	−0.6 (12)
C3—C4—C39—C40	−153.6 (5)	C38—C37—C36—C35	0.8 (13)
C8—C7—C21—C26	110.3 (6)	C17—C18—C19—C20	1.2 (12)
C6—C7—C21—C26	−37.4 (7)	C15—C20—C19—C18	0.4 (11)
C2—C7—C21—C26	−149.5 (5)	C21—C26—C25—C24	−2.2 (12)
C8—C7—C21—C22	−68.7 (7)	C26—C25—C24—C23	3.6 (13)
C6—C7—C21—C22	143.7 (5)	C21—C22—C23—C24	1.0 (14)
C2—C7—C21—C22	31.6 (7)	C25—C24—C23—C22	−3.1 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···Cg1^{i}	0.93	2.91	3.689 (10)	142

Symmetry codes: (i) -x+2, -y, -z.

Fig. 1

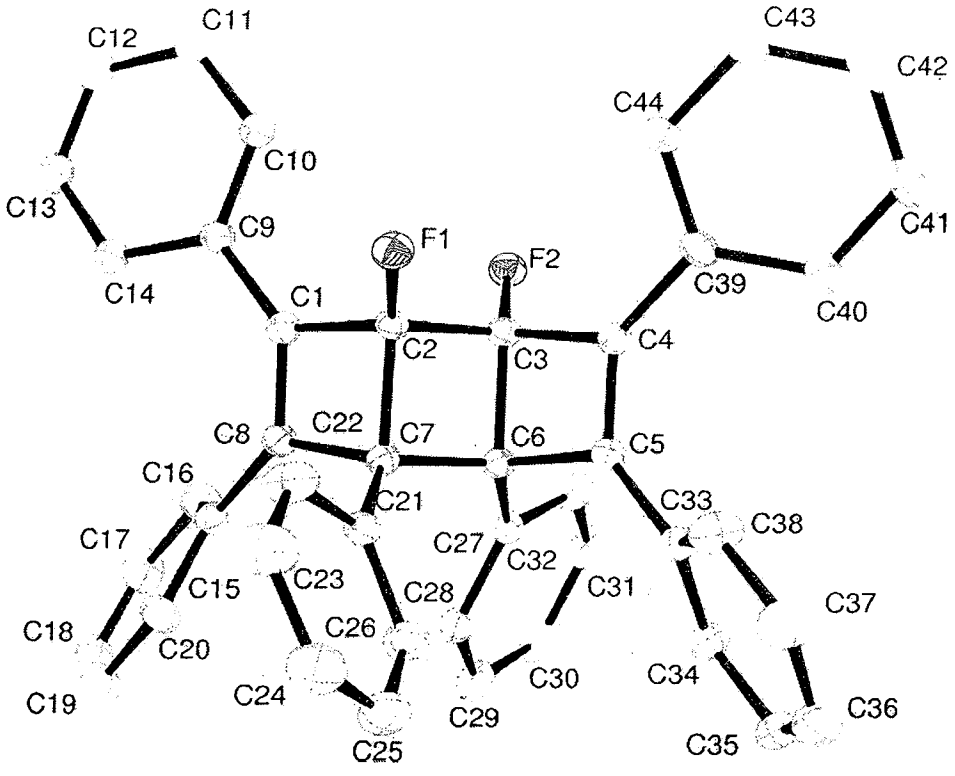

Fig. 2