

1,3,5,7-Tetrakis(4-iodophenyl)-adamantane benzene tetrasolvate

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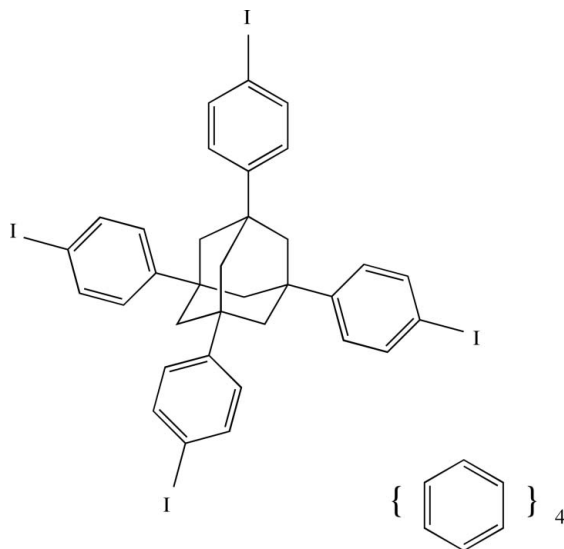
Received 2 June 2010; accepted 7 June 2010

Key indicators: single-crystal X-ray study; $T = 164$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.040; wR factor = 0.105; data-to-parameter ratio = 20.9.

The title molecule, $\text{C}_{34}\text{H}_{28}\text{I}_4 \cdot 4\text{C}_6\text{H}_6$, has crystallographic $\bar{4}$ symmetry and crystallizes with four symmetry-related benzene solvent molecules. The phenyl group is eclipsed with one of the adamantane C—C bonds. The tetraphenyl-adamantane units and the benzene solvent molecules are connected by weak intermolecular phenyl–benzene $\text{C}-\text{H} \cdots \pi$ and benzene–benzene $\text{C}-\text{H} \cdots \pi$ interactions. In the crystal, molecules are linked along the c -axis direction *via* the iodophenyl groups by a combination of weak intermolecular $\text{I} \cdots \text{I}$ [3.944 (1) Å] and $\text{I} \cdots \pi(\text{phenyl})$ [3.608 (6) and 3.692 (5) Å] interactions.

Related literature

For the preparation of the title compound, see: Li *et al.* (2002). For the crystal structure of a related compound, see: Boldog *et al.* (2009). For intermolecular interactions of I atoms, see: Pedireddi *et al.* (1994); Thaimattam *et al.* (1998)



Experimental

Crystal data

$\text{C}_{34}\text{H}_{28}\text{I}_4 \cdot 4\text{C}_6\text{H}_6$
 $M_r = 1256.60$
 Tetragonal, $P\bar{4}2_1c$
 $a = 18.883$ (3) Å
 $c = 7.2442$ (19) Å
 $V = 2583.1$ (9) Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 2.45$ mm⁻¹
 $T = 164$ K
 $0.60 \times 0.20 \times 0.12$ mm

Data collection

Siemens SMART 1K CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2000)
 $T_{\min} = 0.509$, $T_{\max} = 0.751$

35313 measured reflections
 2953 independent reflections
 2365 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.063$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.105$
 $S = 1.05$
 2953 reflections
 141 parameters
 H-atom parameters constrained

$\Delta\rho_{\max} = 1.76$ e Å⁻³
 $\Delta\rho_{\min} = -0.82$ e Å⁻³
 Absolute structure: Flack (1983),
 1263 Friedel pairs
 Flack parameter: -0.01 (4)

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 represent the midpoint of the C13–C14 bond and the centroid of the C10–C15 ring, respectively.

| $D-\text{H} \cdots A$ | $D-\text{H}$ | $\text{H} \cdots A$ | $D \cdots A$ | $D-\text{H} \cdots A$ |
|---|--------------|---------------------|--------------|-----------------------|
| $\text{C5}-\text{H5A} \cdots \text{Cg1}^i$ | 0.95 | 2.91 | 3.833 (9) | 163 |
| $\text{C10}-\text{H10A} \cdots \text{Cg2}^{ii}$ | 0.95 | 2.85 | 3.733 (9) | 156 |

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

Data collection: SMART (Siemens, 1995); cell refinement: SMART; data reduction: SAINT (Siemens, 1995); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXL97.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5063).

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supplementary materials

Acta Cryst. (2010). E66, o1636 [doi:10.1107/S1600536810021744]

1,3,5,7-Tetrakis(4-iodophenyl)adamantane benzene tetrasolvate

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Comment

The title compound was prepared as a precursor for the synthesis of EPR-active tetrahedral model systems.

The asymmetric unit contains a quarter of a 1,3,5,7-tetrakis(4-iodophenyl)adamantane molecule and one benzene solvent molecule. The molecular structure is shown in Fig. 1. The substituted adamantane molecule has $\bar{4}$ symmetry. The conformation of the tetraphenyladamantane unit is very similar to the conformation in the crystal structure of 1,3,5,7-tetraphenyladamantane (Boldog *et al.*, 2009), with the phenyl group eclipsed with one of the adamantane C—C bonds (torsion angle C5—C4—C2—C3ⁱ = 5.7 (6)° [symmetry i: y, 1 - x, 1 - z]).

The crystal packing is shown in Fig. 2. The tetraphenyladamantane and the benzene solvent molecules are connected by intermolecular C—H... π interactions (Table 1, Cg1 and Cg2 represent the midpoint of the C13—C14 bond and the centroid of the C10—C15 ring respectively). There is a C—H... π contact between the phenyl ring and a benzene solvent molecule [angle between planes of rings: 72.9 (2)°]. The C_{phenyl}—H bond does not point to the center of the benzene ring, but closer to the midpoint of the C13—C14 bond. The benzene solvent molecules are connected along the c direction by an additional C—H... π contact. The angle between the planes of the donor and acceptor benzene molecules is 83.3 (2)° and the donor C—H bond points closely to the center of the acceptor ring.

Each C—I bond points to the iodophenyl group of a neighboring molecule as shown in Fig. 3. The shortest contact distances are: I1...I1ⁱ = 3.944 (1) Å, I1...C6ⁱ = 3.608 (6)Å and I1...C7ⁱ = 3.692 (5)Å (symmetry i: 1/2 - y, 1/2 - x, -1/2 + z). The angles for these contacts are: C7—I1...I1ⁱ = 158.6 (1)°, C7—I1...C6ⁱ = 153.9 (2)° and C7—I1...C7ⁱ = 167.0 (2)°. This combination of weak interactions link the 1,3,5,7-tetrakis(4-iodophenyl)adamantane molecules along the c direction. The significance of these interactions for crystal packing has been discussed by Pedireddi *et al.* (1994) and Thaimattam *et al.* (1998).

Experimental

The title compound was prepared as described by Li *et al.* (2002). Single crystals were obtained by recrystallization of the compound from benzene. The crystals rapidly decomposed in the air at room temperature. Therefore a crystal was taken from the mother liquor and was rapidly cooled to 164 K.

Refinement

The H atoms were positioned geometrically and treated as riding: C_{non-planar}—H=0.99 Å, C_{planar}—H=0.95Å and U_{iso}(H)=1.2U_{eq}(C). The absolute structure was determined using 1263 Friedel pairs.

Figures

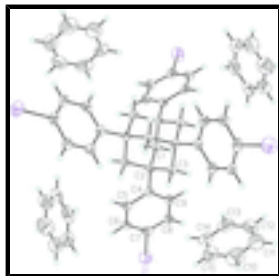


Fig. 1. The structure of the title compound shown with 50% probability displacement ellipsoids. The H atoms are drawn as small spheres of arbitrary radius. Unlabelled atoms are related to labelled atoms by $\bar{4}$ symmetry.

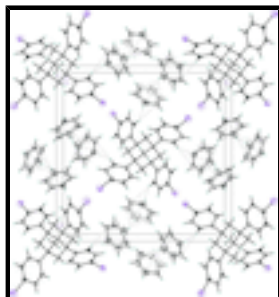


Fig. 2. The crystal packing of the title compound, viewed along the c axis. C—H... π contacts are shown as dotted lines.

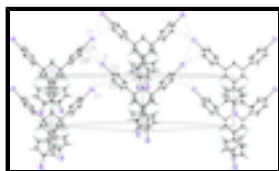


Fig. 3. Section of the crystal structure showing the linking of the 1,3,5,7-tetrakis(4-iodophenyl)adamantane molecules by intermolecular contacts between the iodophenyl groups. The symmetry codes are i: $1/2 - y, 1/2 - x, -1/2 + z$ and ii: $1/2 - y, 1/2 - x, 1/2 + z$.

1,3,5,7-Tetrakis(4-iodophenyl)adamantane benzene tetrasolvate

Crystal data

$C_{34}H_{28}I_4 \cdot 4C_6H_6$
 $M_r = 1256.60$
 Tetragonal, $P\bar{4}2_1c$
 Hall symbol: P -4 2n
 $a = 18.883 (3) \text{ \AA}$
 $c = 7.2442 (19) \text{ \AA}$
 $V = 2583.1 (9) \text{ \AA}^3$
 $Z = 2$
 $F(000) = 1224$

$D_x = 1.616 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 103 reflections
 $\theta = 3\text{--}23^\circ$
 $\mu = 2.45 \text{ mm}^{-1}$
 $T = 164 \text{ K}$
 Rod, colorless
 $0.60 \times 0.20 \times 0.12 \text{ mm}$

Data collection

| | |
|---|---|
| Siemens SMART 1K CCD diffractometer | 2953 independent reflections |
| Radiation source: normal-focus sealed tube graphite | 2365 reflections with $I > 2\sigma(I)$ |
| ω scans | $R_{\text{int}} = 0.063$ |
| Absorption correction: multi-scan | $\theta_{\text{max}} = 27.5^\circ, \theta_{\text{min}} = 1.5^\circ$ |
| | $h = -24 \rightarrow 24$ |

(SADABS; Sheldrick, 2000)

$T_{\min} = 0.509$, $T_{\max} = 0.751$

35313 measured reflections

$k = -24 \rightarrow 24$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.105$

$S = 1.05$

2953 reflections

141 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 1.76 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.82 \text{ e } \text{\AA}^{-3}$

Absolute structure: Flack (1983), 1263 Friedel pairs

Flack parameter: -0.01 (4)

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|-------------|-------------|--------------|----------------------------------|-----------|
| I1 | 0.25295 (2) | 0.30544 (2) | -0.23303 (6) | 0.05317 (17) | |
| C1 | 0.5000 | 0.5000 | 0.2564 (9) | 0.0199 (12) | |
| H1A | 0.5258 | 0.4664 | 0.1760 | 0.024* | 0.50 |
| H1B | 0.4742 | 0.5336 | 0.1760 | 0.024* | 0.50 |
| C2 | 0.4466 (2) | 0.4589 (2) | 0.3747 (6) | 0.0195 (9) | |
| C3 | 0.4875 (3) | 0.4074 (2) | 0.5016 (6) | 0.0209 (9) | |
| H3A | 0.4534 | 0.3815 | 0.5804 | 0.025* | |
| H3B | 0.5129 | 0.3723 | 0.4248 | 0.025* | |
| C4 | 0.3977 (2) | 0.4186 (2) | 0.2437 (6) | 0.0222 (8) | |
| C5 | 0.3250 (2) | 0.4344 (2) | 0.2272 (7) | 0.0274 (10) | |
| H5A | 0.3039 | 0.4677 | 0.3087 | 0.033* | |
| C6 | 0.2844 (3) | 0.4020 (3) | 0.0937 (6) | 0.0287 (11) | |
| H6A | 0.2354 | 0.4131 | 0.0842 | 0.034* | |
| C7 | 0.3139 (3) | 0.3534 (3) | -0.0265 (6) | 0.0310 (11) | |

supplementary materials

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|------|------------|------------|-------------|-------------|
| C8 | 0.3848 (3) | 0.3345 (3) | -0.0094 (7) | 0.0282 (11) |
| H8A | 0.4052 | 0.3000 | -0.0885 | 0.034* |
| C9 | 0.4250 (3) | 0.3675 (3) | 0.1261 (6) | 0.0279 (10) |
| H9A | 0.4734 | 0.3544 | 0.1388 | 0.034* |
| C10 | 0.4526 (5) | 0.1182 (4) | 0.7048 (12) | 0.083 (2) |
| H10A | 0.4384 | 0.0903 | 0.8073 | 0.099* |
| C11 | 0.5184 (5) | 0.1096 (5) | 0.6257 (15) | 0.081 (3) |
| H11A | 0.5501 | 0.0748 | 0.6719 | 0.097* |
| C12 | 0.5372 (4) | 0.1500 (4) | 0.4852 (13) | 0.072 (2) |
| H12A | 0.5831 | 0.1449 | 0.4335 | 0.086* |
| C13 | 0.4918 (4) | 0.1992 (4) | 0.4127 (10) | 0.066 (2) |
| H13A | 0.5055 | 0.2268 | 0.3089 | 0.080* |
| C14 | 0.4265 (4) | 0.2084 (4) | 0.4909 (11) | 0.0612 (19) |
| H14A | 0.3947 | 0.2432 | 0.4445 | 0.073* |
| C15 | 0.4085 (5) | 0.1681 (4) | 0.6319 (14) | 0.078 (3) |
| H15A | 0.3628 | 0.1740 | 0.6849 | 0.094* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|--------------|--------------|--------------|
| I1 | 0.0530 (2) | 0.0577 (3) | 0.0488 (2) | 0.00188 (19) | -0.0243 (2) | -0.0168 (2) |
| C1 | 0.023 (3) | 0.022 (3) | 0.015 (3) | 0.000 (2) | 0.000 | 0.000 |
| C2 | 0.021 (2) | 0.023 (2) | 0.015 (2) | -0.0026 (18) | -0.0018 (17) | -0.0024 (17) |
| C3 | 0.026 (2) | 0.020 (2) | 0.017 (2) | -0.001 (2) | -0.0010 (18) | -0.0001 (17) |
| C4 | 0.026 (2) | 0.026 (2) | 0.015 (2) | -0.0043 (16) | 0.0018 (19) | 0.0027 (19) |
| C5 | 0.029 (2) | 0.024 (2) | 0.029 (2) | -0.0014 (17) | 0.006 (2) | 0.005 (2) |
| C6 | 0.019 (2) | 0.031 (3) | 0.036 (3) | -0.006 (2) | -0.002 (2) | 0.000 (2) |
| C7 | 0.031 (3) | 0.035 (3) | 0.027 (2) | -0.008 (2) | -0.009 (2) | 0.001 (2) |
| C8 | 0.030 (3) | 0.029 (3) | 0.026 (2) | 0.002 (2) | -0.002 (2) | -0.004 (2) |
| C9 | 0.024 (2) | 0.028 (3) | 0.032 (2) | 0.001 (2) | -0.002 (2) | -0.002 (2) |
| C10 | 0.105 (7) | 0.070 (5) | 0.073 (6) | -0.003 (5) | 0.014 (5) | 0.010 (4) |
| C11 | 0.071 (5) | 0.066 (5) | 0.106 (7) | -0.001 (5) | -0.030 (5) | 0.012 (5) |
| C12 | 0.045 (4) | 0.062 (5) | 0.109 (7) | -0.011 (4) | 0.013 (4) | -0.020 (5) |
| C13 | 0.080 (5) | 0.045 (4) | 0.074 (5) | -0.020 (4) | 0.013 (4) | -0.020 (4) |
| C14 | 0.065 (5) | 0.029 (4) | 0.089 (5) | -0.007 (3) | -0.004 (4) | -0.008 (3) |
| C15 | 0.074 (6) | 0.053 (5) | 0.108 (7) | 0.000 (4) | 0.018 (5) | -0.027 (5) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|----------------------|-----------|----------|------------|
| I1—C7 | 2.093 (5) | C7—C8 | 1.391 (7) |
| C1—C2 ⁱ | 1.535 (5) | C8—C9 | 1.388 (6) |
| C1—C2 | 1.535 (5) | C8—H8A | 0.9500 |
| C1—H1A | 0.9900 | C9—H9A | 0.9500 |
| C1—H1B | 0.9900 | C10—C15 | 1.364 (11) |
| C2—C4 | 1.528 (6) | C10—C11 | 1.378 (12) |
| C2—C3 ⁱⁱ | 1.540 (6) | C10—H10A | 0.9500 |
| C2—C3 | 1.545 (6) | C11—C12 | 1.321 (12) |
| C3—C2 ⁱⁱⁱ | 1.540 (6) | C11—H11A | 0.9500 |

| | | | |
|---|------------|-----------------|------------|
| C3—H3A | 0.9900 | C12—C13 | 1.369 (11) |
| C3—H3B | 0.9900 | C12—H12A | 0.9500 |
| C4—C9 | 1.387 (6) | C13—C14 | 1.368 (10) |
| C4—C5 | 1.409 (6) | C13—H13A | 0.9500 |
| C5—C6 | 1.378 (6) | C14—C15 | 1.319 (11) |
| C5—H5A | 0.9500 | C14—H14A | 0.9500 |
| C6—C7 | 1.382 (7) | C15—H15A | 0.9500 |
| C6—H6A | 0.9500 | | |
| C2 ⁱ —C1—C2 | 112.1 (5) | C6—C7—C8 | 120.1 (4) |
| C2 ⁱ —C1—H1A | 109.2 | C6—C7—H1 | 121.1 (4) |
| C2—C1—H1A | 109.2 | C8—C7—H1 | 118.8 (4) |
| C2 ⁱ —C1—H1B | 109.2 | C9—C8—C7 | 118.4 (4) |
| C2—C1—H1B | 109.2 | C9—C8—H8A | 120.8 |
| H1A—C1—H1B | 107.9 | C7—C8—H8A | 120.8 |
| C4—C2—C1 | 107.6 (3) | C4—C9—C8 | 122.8 (4) |
| C4—C2—C3 ⁱⁱ | 113.5 (4) | C4—C9—H9A | 118.6 |
| C1—C2—C3 ⁱⁱ | 107.9 (3) | C8—C9—H9A | 118.6 |
| C4—C2—C3 | 111.0 (4) | C15—C10—C11 | 118.1 (8) |
| C1—C2—C3 | 108.7 (3) | C15—C10—H10A | 120.9 |
| C3 ⁱⁱ —C2—C3 | 107.9 (3) | C11—C10—H10A | 120.9 |
| C2 ⁱⁱⁱ —C3—C2 | 111.9 (4) | C12—C11—C10 | 119.6 (9) |
| C2 ⁱⁱⁱ —C3—H3A | 109.2 | C12—C11—H11A | 120.2 |
| C2—C3—H3A | 109.2 | C10—C11—H11A | 120.2 |
| C2 ⁱⁱⁱ —C3—H3B | 109.2 | C11—C12—C13 | 121.3 (8) |
| C2—C3—H3B | 109.2 | C11—C12—H12A | 119.3 |
| H3A—C3—H3B | 107.9 | C13—C12—H12A | 119.3 |
| C9—C4—C5 | 117.3 (4) | C14—C13—C12 | 119.5 (8) |
| C9—C4—C2 | 120.2 (4) | C14—C13—H13A | 120.3 |
| C5—C4—C2 | 122.4 (4) | C12—C13—H13A | 120.3 |
| C6—C5—C4 | 120.5 (4) | C15—C14—C13 | 118.7 (8) |
| C6—C5—H5A | 119.7 | C15—C14—H14A | 120.7 |
| C4—C5—H5A | 119.7 | C13—C14—H14A | 120.7 |
| C5—C6—C7 | 120.8 (5) | C14—C15—C10 | 122.8 (8) |
| C5—C6—H6A | 119.6 | C14—C15—H15A | 118.6 |
| C7—C6—H6A | 119.6 | C10—C15—H15A | 118.6 |
| C2 ⁱ —C1—C2—C4 | -178.4 (4) | C4—C5—C6—C7 | 0.0 (7) |
| C2 ⁱ —C1—C2—C3 ⁱⁱ | 58.7 (3) | C5—C6—C7—C8 | 2.5 (7) |
| C2 ⁱ —C1—C2—C3 | -58.1 (3) | C5—C6—C7—H1 | -178.8 (3) |
| C4—C2—C3—C2 ⁱⁱⁱ | 175.9 (4) | C6—C7—C8—C9 | -2.3 (7) |
| C1—C2—C3—C2 ⁱⁱⁱ | 57.7 (5) | H1—C7—C8—C9 | 179.0 (3) |
| C3 ⁱⁱ —C2—C3—C2 ⁱⁱⁱ | -59.1 (3) | C5—C4—C9—C8 | 2.9 (7) |
| C1—C2—C4—C9 | 61.9 (5) | C2—C4—C9—C8 | -172.9 (4) |
| C3 ⁱⁱ —C2—C4—C9 | -178.8 (4) | C7—C8—C9—C4 | -0.5 (7) |
| C3—C2—C4—C9 | -57.0 (5) | C15—C10—C11—C12 | 1.1 (14) |
| C1—C2—C4—C5 | -113.7 (4) | C10—C11—C12—C13 | -1.9 (13) |

supplementary materials

| | | | |
|----------------------------|-----------|-----------------|-----------|
| C3 ⁱⁱ —C2—C4—C5 | 5.7 (6) | C11—C12—C13—C14 | 2.2 (12) |
| C3—C2—C4—C5 | 127.4 (4) | C12—C13—C14—C15 | -1.7 (11) |
| C9—C4—C5—C6 | -2.6 (6) | C13—C14—C15—C10 | 0.9 (12) |
| C2—C4—C5—C6 | 173.1 (4) | C11—C10—C15—C14 | -0.6 (13) |

Symmetry codes: (i) $-x+1, -y+1, z$; (ii) $y, -x+1, -z+1$; (iii) $-y+1, x, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

$Cg1$ and $Cg2$ represent the midpoint of the C13—C14 bond and the centroid of the C10—C15 ring, respectively.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------------------|-------|-------------|-------------|---------------|
| C5—H5A \cdots Cg1 ⁱⁱ | 0.95 | 2.91 | 3.833 (9) | 163 |
| C10—H10A \cdots Cg2 ^{iv} | 0.95 | 2.85 | 3.733 (9) | 156 |

Symmetry codes: (ii) $y, -x+1, -z+1$; (iv) $-y+1/2, -x+1/2, z+1/2$.

Fig. 1

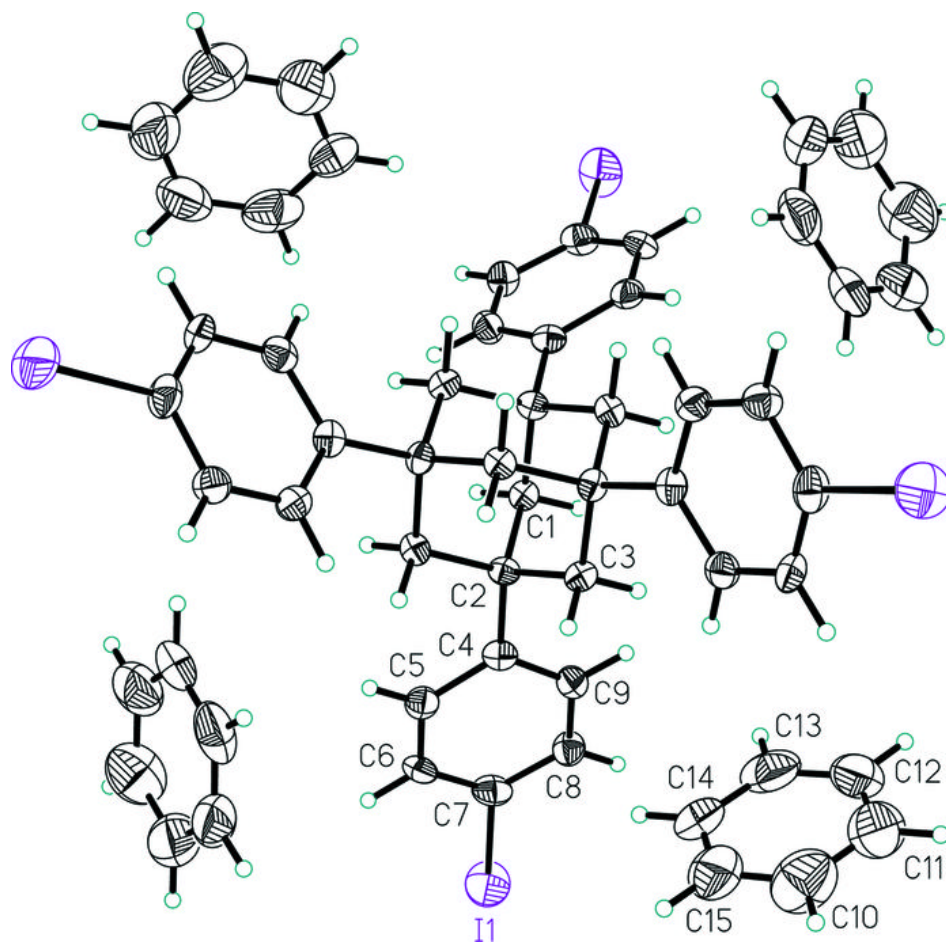


Fig. 2

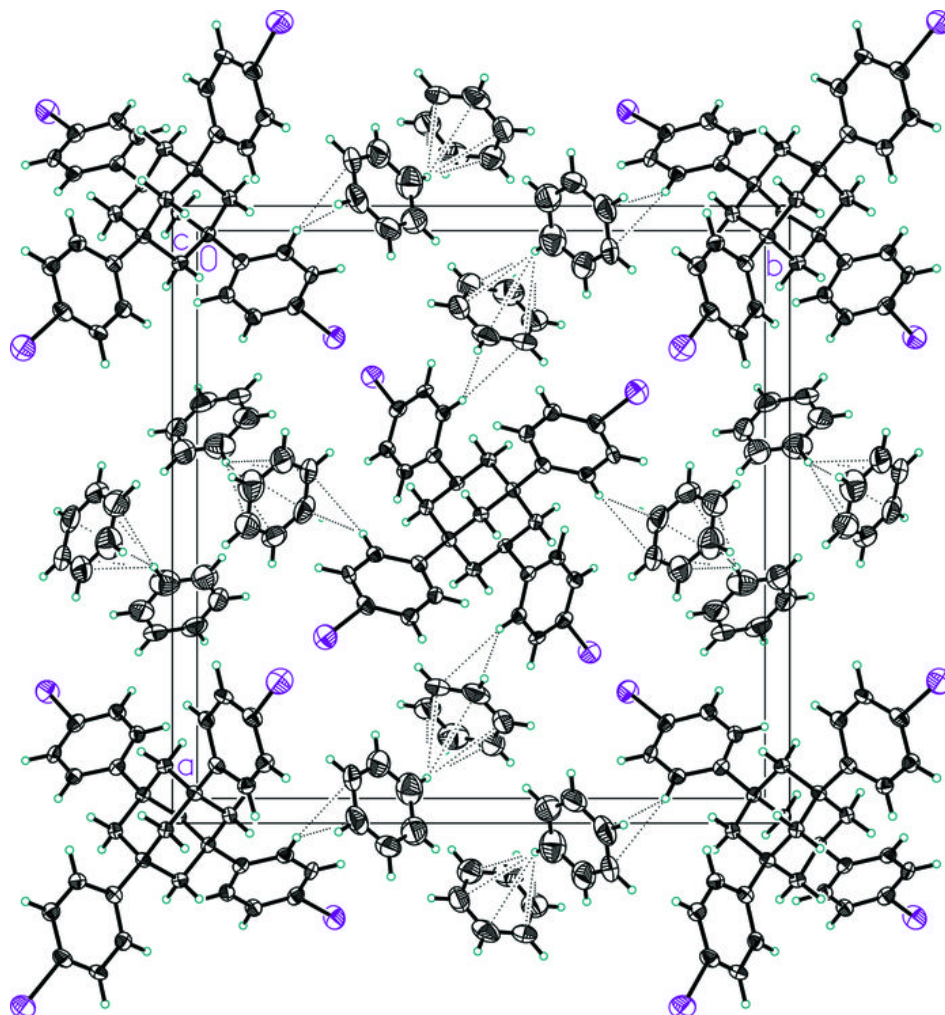


Fig. 3

