

Philippe Fernandes,^a Alastair
Florence,^{a*} Kenneth Shankland^b
and William I. F. David^b^aDepartment of Pharmaceutical Sciences,
University of Strathclyde, 27 Taylor Street,
Glasgow G4 0NR, Scotland, and ^bBISIS Facility,
Rutherford Appleton Laboratory, Chilton,
Didcot, Oxfordshire OX11 0QX, EnglandCorrespondence e-mail:
alastair.florence@strath.ac.uk**Key indicators**

Powder X-ray study

 $T = 295$ KMean $\sigma(\text{C}-\text{C}) = 0.092$ Å R factor = 0.036 wR factor = 0.036

Data-to-parameter ratio = 3.1

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**Powder diffraction study of 1,2:3,4-
dibenzanthracene**

The crystal structure of 1,2:3,4-dibenzanthracene, $\text{C}_{22}\text{H}_{14}$, was solved by simulated annealing from laboratory X-ray powder diffraction data collected at room temperature to 1.8 Å resolution. Subsequent Rietveld refinement yielded an R_{wp} value of 0.036. The molecules crystallize in space group $P2_1$ with two independent molecules in the asymmetric unit which pack in a stacked arrangement along the b axis.

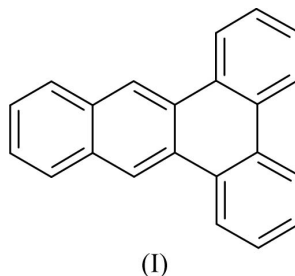
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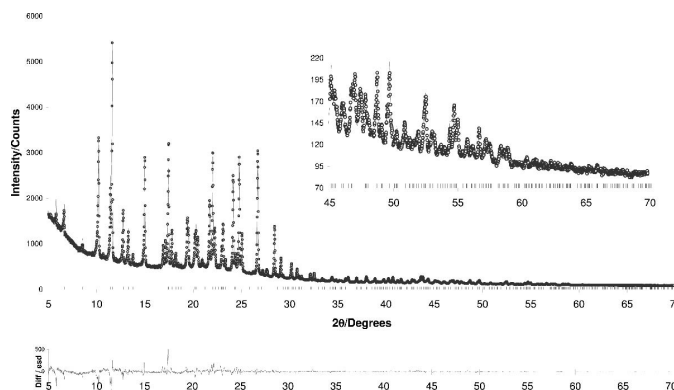
Online 27 April 2005

Comment

The title compound, (I), was used as supplied and its crystal structure was solved by simulated annealing using laboratory X-ray powder diffraction data (Fig. 1). The compound crystallizes in space group $P2_1$ with two independent molecules in the asymmetric unit (Fig. 2).



The crystal packing adopts a γ -type structure, with molecules stacked in the direction of the b axis (Desiraju & Gavezzotti, 1989). The distance between the centres of mass of neighbouring molecules within each stack (R_n) equals the shortest cell axis, 5.062 Å, and the perpendicular distance between the molecular planes within each stack (R_{ip}) is 3.740 Å, with an offset angle $\alpha = 43^\circ$ (Fig. 3).

**Figure 1**

Final observed (points), calculated (line) and difference $[(y_{\text{obs}} - y_{\text{calc}})/\sigma(y_{\text{obs}})]$ profiles for the Rietveld refinement of (I).

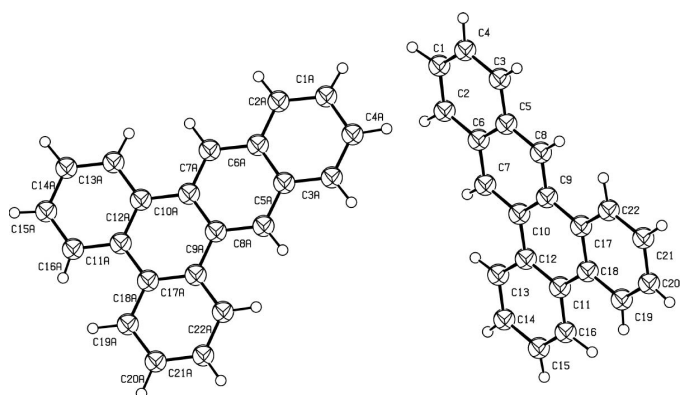


Figure 2

The atomic arrangement in (I), showing the two molecules in the asymmetric unit. The dihedral angle between the least-squares planes through each of the molecules is $47.8(8)^\circ$. Isotropic displacement spheres are shown at the 50% probability level.

Experimental

1,2,3,4-Dibenzanthracene (Sigma–Aldrich) was lightly ground in a mortar, loaded into a 0.7 mm borosilicate glass capillary and mounted on the diffractometer. Data were collected from a sample in a rotating 0.7 mm borosilicate glass capillary using a variable count time scheme (Hill & Madsen, 2002).

Crystal data

$C_{22}H_{14}$
 $M_r = 278.33$
 Monoclinic, $P2_1$
 $a = 18.2966(5) \text{ \AA}$
 $b = 5.06225(10) \text{ \AA}$
 $c = 15.7245(4) \text{ \AA}$
 $\beta = 104.5574(15)^\circ$
 $V = 1409.68(6) \text{ \AA}^3$
 $Z = 4$

$D_x = 1.311 \text{ Mg m}^{-3}$
 Cu $K\alpha_1$ radiation
 $\mu = 0.56 \text{ mm}^{-1}$
 $T = 295 \text{ K}$
 Specimen shape: cylinder
 $12 \times 0.7 \text{ mm}$
 Specimen prepared at 295 K
 Particle morphology: visual estimate, flat plate, pale yellow

Data collection

Bruker D8 Advance diffractometer
 Specimen mounting: 0.7 mm borosilicate capillary
 Specimen mounted in transmission mode
 Scan method: step

Absorption correction: none
 $2\theta_{\min} = 4$, $2\theta_{\max} = 69.8^\circ$
 Increment in $2\theta = 0.014^\circ$
 $h = -13 \rightarrow 13$
 $k = -3 \rightarrow 3$
 $l = -9 \rightarrow 11$

Refinement

Refinement on F^2
 $R_p = 0.036$
 $R_{wp} = 0.036$
 $R_{exp} = 0.014$
 $S = 2.69$
 Increment in $2\theta = 0.014^\circ$
 Wavelength of incident radiation: 1.54056 \AA
 Profile function: fundamental parameters with axial divergence correction

739 reflections
 241 parameters
 Only H-atom coordinates refined
 $w = 1/\sigma(y_{obs})^2$
 $(\Delta/\sigma)_{\max} = 0.011$
 Preferred orientation correction: a spherical harmonics-based preferred orientation correction was applied with *TOPAS* during the Rietveld refinement.

The diffraction pattern indexed to a monoclinic cell [$F(25) = 210.1$, $M(25) = 71.8$; *DICVOL-91* (Boultif & Louer, 1991)], and space group $P2_1$ was assigned from volume considerations and a statistical consideration of the systematic absences. The data set was background-subtracted and truncated to $2\theta = 51.9^\circ$ for Pawley fitting (Pawley, 1981; $\chi^2_{Pawley} = 3.96$), and the structure was solved using the simulated annealing (SA) global optimization procedure of David *et*

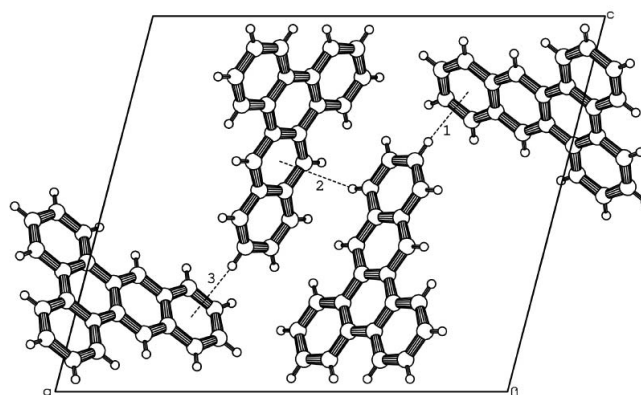
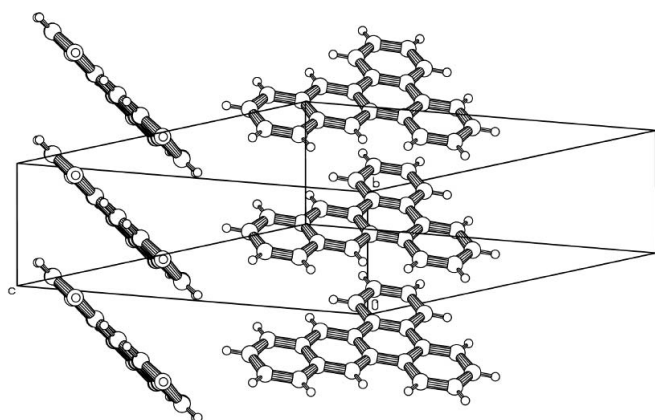


Figure 3

Top: view showing the molecular stacking along the b axis in (I) for both unique molecules. Molecules within each stack form offset face-to-face attractive contacts (Hunter *et al.*, 1990). Bottom: view down the b axis onto the ac plane. The crystal packing arrangement is stabilized by a series of $C-H \cdots \pi$ contacts between adjacent stacks, with $H \cdots$ ring-centroid (C_g) distances in the range 2.9(5)–3.3(5) Å. Dashed lines represent three of these contacts. (1) $C4A-H26A \cdots C_g$ of the ring $C1-C6$ in the molecule at $(x, 1+y, z)$ [$H26A \cdots C_g$ 2.9(5) Å], (2) $C2A-H24A \cdots C_g$ of the ring $C5A-C10A$ in the molecule at $(1-x, \frac{1}{2}+y, 1-z)$ [$H24A \cdots C_g$ 3.2(6) Å] and (3) the symmetry equivalent of (1), where $H26A$ and C_g are in the molecules at $(1-x, \frac{1}{2}+y, 1-z)$.

al. (1998), as implemented in the *DASH* computer program (David *et al.*, 2001). The SA structure solution involved the optimization of two independent fragments in the asymmetric unit, totalling 12 degrees of freedom. The best SA solution had a favourable $\chi^2_{SA}/\chi^2_{Pawley}$ ratio of 4.53 and a chemically reasonable packing arrangement, and exhibited no significant misfit to the data. The solved structure was then refined with the full data set (2θ 4–69.8°) using a restrained Rietveld method (Rietveld, 1969), as implemented in *TOPAS* (Coelho, 2003), with the value of R_{wp} falling from 0.146 to 0.036 during the refinement. The y coordinate of atom $C1$ was fixed and all remaining atomic positions (including H atoms) were refined, subject to a series of restraints on bond lengths, bond angles and planarity. Inclusion of a March–Dollase (Dollase, 1986) preferred orientation correction indicated the presence of mild (1.16) preferred orientation along the $[010]$ direction, and a spherical harmonics correction of intensities for

preferred orientation was applied in the final refinement. The observed and calculated diffraction patterns for the refined crystal structure are shown in Fig. 1.

Data collection: *DIFFRAC* plus *XRD Commander* (Kienle & Jacob, 2003); cell refinement: *TOPAS* (Coelho, 2003); data reduction: *DASH* (David *et al.*, 2001); structure solution: *DASH*; structure refinement: *TOPAS*; molecular graphics: *PLATON* (Spek, 2003); publication software: *enCIFer* (Allen *et al.*, 2004).

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supporting information

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Powder diffraction study of 1,2:3,4-dibenzanthracene

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1,2:5,6-Dibenzanthracene

Crystal data

$C_{22}H_{14}$

$M_r = 278.33$

Monoclinic, $P2_1$

Hall symbol: P 2_yb

$a = 18.2966$ (5) Å

$b = 5.06225$ (10) Å

$c = 15.7245$ (4) Å

$\beta = 104.5574$ (15)°

$V = 1409.68$ (6) Å³

$Z = 4$

$F(000) = 584$

$D_x = 1.311$ Mg m⁻³

Melting point: 500 K

Cu $K\alpha 1$ radiation, $\lambda = 1.54056$ Å

$\mu = 0.56$ mm⁻¹

$T = 295$ K

Particle morphology: visual estimate, flat plates

pale-yellow

cylinder, 10 × 0.7 mm

Specimen preparation: Prepared at 295 K

Data collection

Bruker D8 Advance
diffractometer

Radiation source: sealed X-ray tube, Bruker D8

Primary focussing, Ge 111 monochromator

Specimen mounting: 0.7 mm borosilicate
capillary

Data collection mode: transmission

Scan method: step

$2\theta_{\min} = 4^\circ$, $2\theta_{\max} = 69.8^\circ$, $2\theta_{\text{step}} = 0.014^\circ$

Refinement

Least-squares matrix: selected elements only

$R_p = 0.036$

$R_{wp} = 0.036$

$R_{\text{exp}} = 0.014$

4544 data points

Profile function: Fundamental parameters with
axial divergence correction

241 parameters

214 restraints

1 constraint

Only H-atom coordinates refined

Weighting scheme based on measured s.u.'s

$1/\sigma(Y_{\text{obs}})^2$

$(\Delta/\sigma)_{\max} = 0.011$

Background function: Chebyshev polynomial

Preferred orientation correction: A spherical
harmonics-based preferred orientation
correction was applied with TOPAS during the
Rietveld refinement.

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All e.s.d.'s are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.305 (3)	-0.06763	0.781 (5)	0.0465 (10)*

C2	0.235 (3)	-0.011 (17)	0.724 (3)	0.0465 (10)*
C3	0.283 (3)	0.274 (16)	0.880 (3)	0.0465 (10)*
C4	0.331 (2)	0.085 (17)	0.857 (3)	0.0465 (10)*
C5	0.211 (3)	0.323 (15)	0.824 (3)	0.0465 (10)*
C6	0.187 (3)	0.179 (16)	0.746 (4)	0.0465 (10)*
C7	0.115 (3)	0.228 (15)	0.690 (3)	0.0465 (10)*
C8	0.163 (3)	0.513 (13)	0.847 (3)	0.0465 (10)*
C9	0.092 (3)	0.562 (14)	0.791 (4)	0.0465 (10)*
C10	0.067 (3)	0.419 (14)	0.712 (3)	0.0465 (10)*
C11	-0.052 (3)	0.658 (16)	0.679 (4)	0.0465 (10)*
C12	-0.005 (3)	0.467 (17)	0.656 (4)	0.0465 (10)*
C13	-0.029 (3)	0.323 (16)	0.578 (4)	0.0465 (10)*
C14	-0.100 (3)	0.372 (16)	0.522 (3)	0.0465 (10)*
C15	-0.148 (3)	0.561 (16)	0.545 (4)	0.0465 (10)*
C16	-0.123 (3)	0.706 (16)	0.622 (4)	0.0465 (10)*
C17	0.044 (3)	0.752 (17)	0.813 (4)	0.0465 (10)*
C18	-0.028 (3)	0.801 (14)	0.757 (4)	0.0465 (10)*
C19	-0.075 (3)	0.991 (18)	0.780 (4)	0.0465 (10)*
C20	-0.050 (3)	1.136 (17)	0.858 (4)	0.0465 (10)*
C21	0.021 (3)	1.084 (17)	0.915 (3)	0.0465 (10)*
C22	0.068 (3)	0.896 (16)	0.891 (4)	0.0465 (10)*
H23	0.34 (3)	-0.19 (11)	0.76 (3)	0.0760*
H24	0.22 (3)	-0.11 (9)	0.67 (3)	0.0760*
H25	0.30 (3)	0.37 (11)	0.93 (2)	0.0760*
H26	0.38 (2)	0.05 (10)	0.90 (3)	0.0760*
H27	0.10 (3)	0.13 (10)	0.64 (3)	0.0760*
H28	0.18 (2)	0.61 (12)	0.90 (3)	0.0760*
H29	0.00 (2)	0.20 (11)	0.56 (3)	0.0760*
H30	-0.12 (2)	0.28 (9)	0.47 (3)	0.0760*
H31	-0.196 (17)	0.59 (8)	0.51 (3)	0.0760*
H32	-0.16 (2)	0.83 (9)	0.64 (3)	0.0760*
H33	-0.12 (2)	1.03 (12)	0.74 (3)	0.0760*
H34	-0.08 (2)	1.26 (10)	0.87 (3)	0.0760*
H35	0.04 (3)	1.18 (12)	0.97 (3)	0.0760*
H36	0.12 (2)	0.86 (9)	0.93 (3)	0.0760*
C1A	0.393 (3)	0.174 (16)	0.616 (3)	0.0465 (10)*
C2A	0.421 (3)	0.133 (15)	0.542 (4)	0.0465 (10)*
C3A	0.308 (3)	0.511 (18)	0.538 (4)	0.0465 (10)*
C4A	0.337 (3)	0.364 (18)	0.614 (3)	0.0465 (10)*
C5A	0.335 (3)	0.470 (15)	0.463 (3)	0.0465 (10)*
C6A	0.391 (3)	0.281 (15)	0.465 (4)	0.0465 (10)*
C7A	0.419 (3)	0.240 (17)	0.390 (5)	0.0465 (10)*
C8A	0.306 (3)	0.618 (17)	0.387 (4)	0.0465 (10)*
C9A	0.333 (3)	0.577 (15)	0.312 (4)	0.0465 (10)*
C10A	0.389 (3)	0.388 (17)	0.313 (3)	0.0465 (10)*
C11A	0.386 (3)	0.498 (19)	0.161 (4)	0.0465 (10)*
C12A	0.416 (3)	0.349 (16)	0.237 (4)	0.0465 (10)*
C13A	0.472 (3)	0.159 (16)	0.237 (3)	0.0465 (10)*

C14A	0.499 (3)	0.122 (17)	0.163 (4)	0.0465 (10)*
C15A	0.469 (3)	0.271 (16)	0.087 (4)	0.0465 (10)*
C16A	0.413 (3)	0.460 (15)	0.086 (4)	0.0465 (10)*
C17A	0.303 (3)	0.726 (16)	0.236 (3)	0.0465 (10)*
C18A	0.330 (3)	0.687 (15)	0.161 (4)	0.0465 (10)*
C19A	0.300 (3)	0.838 (16)	0.085 (4)	0.0465 (10)*
C20A	0.244 (3)	1.027 (17)	0.086 (3)	0.0465 (10)*
C21A	0.217 (3)	1.063 (17)	0.161 (5)	0.0465 (10)*
C22A	0.247 (3)	0.91 (2)	0.236 (4)	0.0465 (10)*
H23A	0.41 (2)	0.08 (10)	0.67 (2)	0.0760*
H24A	0.46 (3)	0.01 (11)	0.54 (3)	0.0760*
H25A	0.27 (2)	0.64 (9)	0.54 (3)	0.0760*
H26A	0.32 (2)	0.39 (11)	0.67 (3)	0.0760*
H27A	0.46 (2)	0.11 (10)	0.39 (3)	0.0760*
H28A	0.27 (2)	0.75 (11)	0.39 (3)	0.0760*
H29A	0.49 (2)	0.06 (9)	0.29 (2)	0.0760*
H30A	0.54 (2)	-0.01 (10)	0.16 (3)	0.0760*
H31A	0.49 (2)	0.24 (11)	0.04 (3)	0.0760*
H32A	0.39 (3)	0.56 (10)	0.04 (2)	0.0760*
H33A	0.32 (2)	0.81 (10)	0.03 (3)	0.0760*
H34A	0.22 (2)	1.13 (9)	0.03 (3)	0.0760*
H35A	0.18 (2)	1.19 (11)	0.16 (3)	0.0760*
H36A	0.23 (2)	0.94 (12)	0.29 (3)	0.0760*

Geometric parameters (Å, °)

C1—C2	1.40 (9)	C1A—C2A	1.40 (8)
C1—C4	1.40 (9)	C1A—C4A	1.40 (10)
C2—C6	1.40 (10)	C2A—C6A	1.41 (9)
C3—C4	1.41 (9)	C3A—C4A	1.39 (9)
C3—C5	1.41 (8)	C3A—C5A	1.40 (8)
C5—C6	1.40 (9)	C5A—C6A	1.40 (9)
C5—C8	1.41 (9)	C5A—C8A	1.40 (9)
C6—C7	1.41 (8)	C6A—C7A	1.41 (9)
C7—C10	1.41 (9)	C7A—C10A	1.41 (10)
C8—C9	1.41 (8)	C8A—C9A	1.40 (9)
C9—C10	1.41 (8)	C9A—C10A	1.40 (10)
C9—C17	1.39 (10)	C9A—C17A	1.40 (9)
C10—C12	1.40 (8)	C10A—C12A	1.42 (7)
C11—C12	1.41 (10)	C11A—C12A	1.40 (10)
C11—C16	1.40 (8)	C11A—C16A	1.40 (9)
C11—C18	1.40 (9)	C11A—C18A	1.40 (10)
C12—C13	1.40 (10)	C12A—C13A	1.41 (9)
C13—C14	1.40 (8)	C13A—C14A	1.38 (8)
C14—C15	1.41 (10)	C14A—C15A	1.40 (10)
C15—C16	1.39 (9)	C15A—C16A	1.40 (10)
C17—C18	1.40 (8)	C17A—C18A	1.40 (8)
C17—C22	1.40 (10)	C17A—C22A	1.38 (11)

C18—C19	1.41 (10)	C18A—C19A	1.41 (9)
C19—C20	1.40 (10)	C19A—C20A	1.40 (10)
C20—C21	1.41 (8)	C20A—C21A	1.40 (9)
C21—C22	1.40 (10)	C21A—C22A	1.40 (11)
C1—H23	1.0 (5)	C1A—H23A	1.0 (3)
C2—H24	1.0 (4)	C2A—H24A	1.0 (5)
C3—H25	0.9 (5)	C3A—H25A	1.0 (4)
C4—H26	0.9 (5)	C4A—H26A	1.0 (5)
C7—H27	0.9 (4)	C7A—H27A	1.0 (4)
C8—H28	0.9 (6)	C8A—H28A	0.9 (5)
C13—H29	0.9 (4)	C13A—H29A	1.0 (3)
C14—H30	0.9 (4)	C14A—H30A	1.0 (4)
C15—H31	0.9 (3)	C15A—H31A	0.9 (4)
C16—H32	1.0 (5)	C16A—H32A	0.9 (4)
C19—H33	0.9 (4)	C19A—H33A	1.0 (4)
C20—H34	0.9 (5)	C20A—H34A	1.0 (4)
C21—H35	1.0 (6)	C21A—H35A	0.9 (5)
C22—H36	1.0 (5)	C22A—H36A	1.0 (5)
C2—C1—C4	120 (5)	C2A—C1A—C4A	120 (5)
C1—C2—C6	121 (5)	C1A—C2A—C6A	119 (6)
C4—C3—C5	120 (5)	C4A—C3A—C5A	120 (6)
C1—C4—C3	120 (4)	C1A—C4A—C3A	120 (5)
C3—C5—C6	120 (6)	C3A—C5A—C6A	120 (6)
C3—C5—C8	120 (5)	C3A—C5A—C8A	120 (6)
C6—C5—C8	120 (5)	C6A—C5A—C8A	120 (5)
C2—C6—C5	120 (5)	C2A—C6A—C5A	121 (5)
C2—C6—C7	121 (6)	C2A—C6A—C7A	120 (6)
C5—C6—C7	120 (6)	C5A—C6A—C7A	120 (6)
C6—C7—C10	121 (5)	C6A—C7A—C10A	120 (6)
C5—C8—C9	120 (5)	C5A—C8A—C9A	120 (6)
C8—C9—C10	120 (6)	C8A—C9A—C10A	120 (6)
C8—C9—C17	120 (6)	C8A—C9A—C17A	119 (6)
C10—C9—C17	120 (5)	C10A—C9A—C17A	120 (5)
C7—C10—C9	120 (5)	C7A—C10A—C9A	120 (5)
C7—C10—C12	120 (5)	C7A—C10A—C12A	120 (6)
C9—C10—C12	120 (6)	C9A—C10A—C12A	120 (6)
C12—C11—C16	119 (6)	C12A—C11A—C16A	120 (7)
C12—C11—C18	119 (5)	C12A—C11A—C18A	120 (5)
C16—C11—C18	121 (6)	C16A—C11A—C18A	120 (6)
C10—C12—C11	120 (6)	C10A—C12A—C11A	120 (6)
C10—C12—C13	121 (6)	C10A—C12A—C13A	120 (6)
C11—C12—C13	120 (6)	C11A—C12A—C13A	120 (5)
C12—C13—C14	120 (6)	C12A—C13A—C14A	120 (6)
C13—C14—C15	120 (5)	C13A—C14A—C15A	121 (6)
C14—C15—C16	120 (5)	C14A—C15A—C16A	120 (6)
C11—C16—C15	121 (6)	C11A—C16A—C15A	120 (6)
C9—C17—C18	120 (6)	C9A—C17A—C18A	120 (6)

C9—C17—C22	120 (6)	C9A—C17A—C22A	120 (5)
C18—C17—C22	120 (6)	C18A—C17A—C22A	121 (6)
C11—C18—C17	121 (6)	C11A—C18A—C17A	121 (6)
C11—C18—C19	119 (6)	C11A—C18A—C19A	120 (6)
C17—C18—C19	120 (6)	C17A—C18A—C19A	120 (6)
C18—C19—C20	120 (6)	C18A—C19A—C20A	119 (5)
C19—C20—C21	120 (7)	C19A—C20A—C21A	121 (6)
C20—C21—C22	119 (6)	C20A—C21A—C22A	119 (7)
C17—C22—C21	121 (5)	C17A—C22A—C21A	120 (6)
C2—C1—H23	118	C2A—C1A—H23A	124
C4—C1—H23	121	C4A—C1A—H23A	116
C1—C2—H24	118	C1A—C2A—H24A	124
C6—C2—H24	121	C6A—C2A—H24A	117
C4—C3—H25	119	C4A—C3A—H25A	117
C5—C3—H25	121	C5A—C3A—H25A	123
C1—C4—H26	122	C1A—C4A—H26A	117
C3—C4—H26	118	C3A—C4A—H26A	123
C6—C7—H27	118	C6A—C7A—H27A	122
C10—C7—H27	121	C10A—C7A—H27A	119
C5—C8—H28	119	C5A—C8A—H28A	117
C9—C8—H28	120	C9A—C8A—H28A	123
C12—C13—H29	123	C12A—C13A—H29A	117
C14—C13—H29	117	C14A—C13A—H29A	123
C13—C14—H30	124	C13A—C14A—H30A	123
C15—C14—H30	116	C15A—C14A—H30A	116
C14—C15—H31	121	C14A—C15A—H31A	116
C16—C15—H31	119	C16A—C15A—H31A	124
C11—C16—H32	120	C11A—C16A—H32A	114
C15—C16—H32	118	C15A—C16A—H32A	126
C18—C19—H33	119	C18A—C19A—H33A	120
C20—C19—H33	121	C20A—C19A—H33A	121
C19—C20—H34	118	C19A—C20A—H34A	120
C21—C20—H34	121	C21A—C20A—H34A	120
C20—C21—H35	123	C20A—C21A—H35A	119
C22—C21—H35	118	C22A—C21A—H35A	122
C17—C22—H36	119	C17A—C22A—H36A	120
C21—C22—H36	121	C21A—C22A—H36A	120
