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5,10-Dihydroindeno[2,1-*a*]indene

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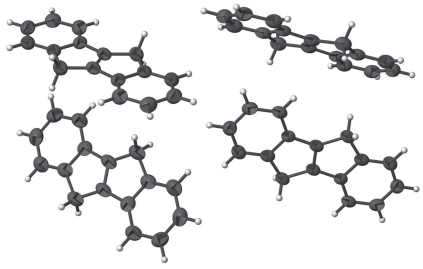
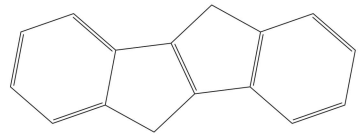
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{16}H_{12}$, crystallizes with four half molecules in the asymmetric unit, each of which is located on a crystallographic centre of inversion. The molecules are essentially planar. The crystal studied was a non-merohedral twin.

3D view



Chemical scheme



Structure description

Indenoindene is well known as starting material for *e.g.* pentalenes (Frank & Gompper, 1987) and has been studied as a stiffened stilbene (Ogawa *et al.*, 1988; Krohn *et al.*, 2019). While the compound is formed in pyrolytic processes (Hofmann *et al.*, 1995), synthetic routes involve benzocyclobutene derivatives (Barton & Shepherd 1987; Schiess & Heitzmann 1977; Detert & Schollmeyer 2018) and a photochemical rearrangement (Oelgemöller *et al.*, 2002).

Four independent and nearly identical molecules of the title compound with essential C_{2h} symmetry fill the unit cell (Fig. 1). The crystal packing shows pairs of tilted molecules along the *a* axis and along the *b* axis (Fig. 2). The molecules are completely planar [maximum deviation from the mean plane of all carbon atoms in a molecule: 0.014 (3) Å for C6*D*]. The central dihydropentalene unit shows averaged bond lengths of 1.466 (4) Å for C2—C3 and 1.331 (4) Å for C2—C2′. A comparison of these data with *trans* stilbene (1.466 and 1.324 Å, respectively; Luo *et al.*, 2019) reveals a bond-length convergence in the planarized indenoindene [dihedral angle = 1.2 (2)°] relative to the twisted stilbene (phenylethenyl torsion angle = 6.64°)

Synthesis and crystallization

The title compound was prepared according to Oelgemöller *et al.* (2002). Single crystals were obtained by slow evaporation of a solution in dichloromethane/propanol-2 (2:1).

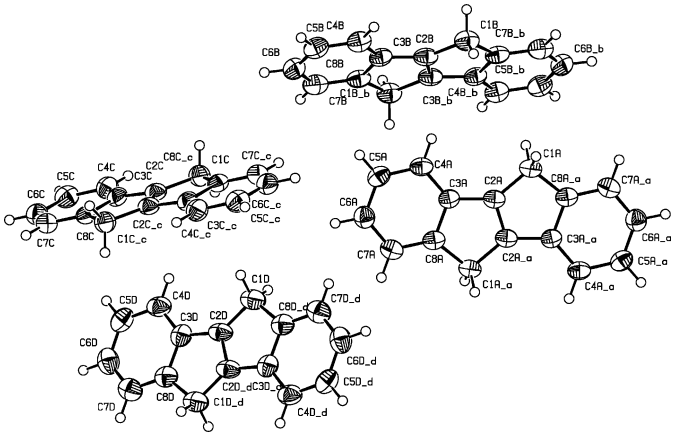


Figure 1
Perspective view of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The crystal studied was a non-merohedral two-component twin with a fractional contribution of 0.4085 (12) for the minor domain.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{12}$
M_r	204.26
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	193
a, b, c (Å)	7.5009 (9), 7.6819 (9), 19.387 (3)
α, β, γ (°)	99.733 (11), 100.641 (11), 90.523 (9)
V (Å^3)	1081.2 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.22 × 0.15 × 0.04
Data collection	
Diffractometer	Stoe *IPDS* 2T
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14443, 14443, 7500
R_{int}	?
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.141, 1.03
No. of reflections	14443
No. of parameters	290
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.21

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 1996), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2009).

Acknowledgements

The authors are grateful to N. Jacobs for the preparation of the title compound.

References

Barton, J. W. & Shepherd, M. K. (1987). *J. Chem. Soc. Perkin Trans. 1*, pp. 1561–1565.
Detert, H. & Schollmeyer, D. (2018). *IUCrData*, **3**, x181550.
Frank, W. & Gompper, R. (1987). *Tetrahedron Lett.* **28**, 3083–3086.
Hofmann, J., Zimmermann, G., Guthier, K., Hebgen, P. & Homann, K.-H. (1995). *Liebigs Ann.* , pp. 631–636.
Krohn, O. A., Quick, M., Ioffe, I. N., Mazaleva, O. N., Lenoir, D., Detert, H. & Kovalenko, S. A. (2019). *J. Phys. Chem. B*, **123**, 4291–4300.
Luo, X., Chen, X., Chen, L., Zhang, K. & Li, Y. (2019). *Chem. Commun.* **55** 20170–20173.
Oelgemöller, M., Brem, B., Frank, R., Schneider, S., Lenoir, D., Hertkorn, N., Origane, Y., Lemmen, P., Lex, J. & Inoue, Y. (2002). *J. Chem. Soc. Perkin Trans. 2*, pp. 1760–1771.
Ogawa, K., Futakami, M., Suzuki, H. & Kira, A. (1988). *J. Chem. Soc. Perkin Trans. 2*, pp. 2115–2118.
Schiess, P. & Heitzmann, M. (1977). *Angew. Chem.* **89**, 485–485.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Stoe & Cie (1996). *X-RED* and *X-AREA*. Stoe & Cie, Darmstadt, Germany.

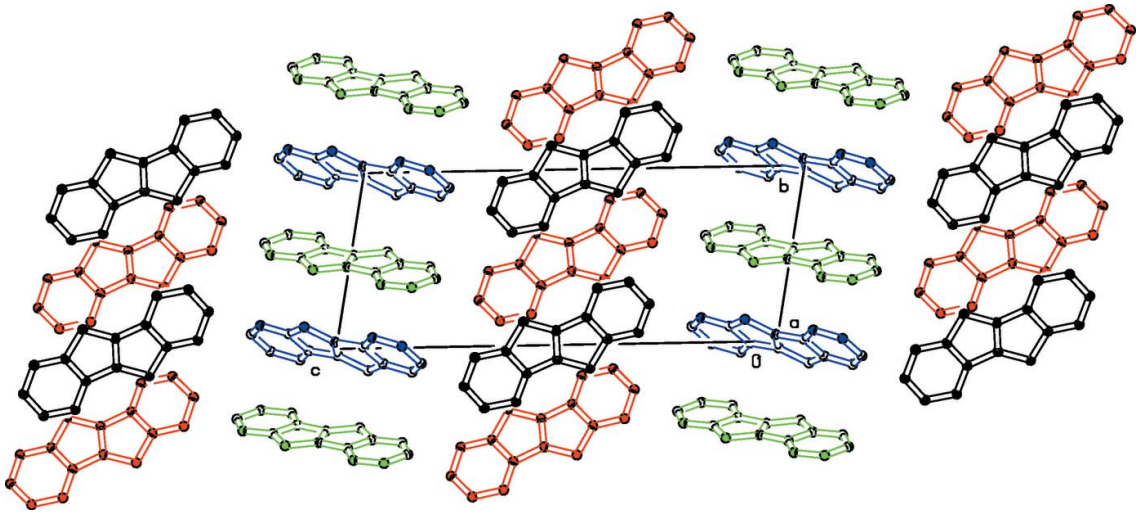


Figure 2
Packing diagram of the title compound viewed along the *a* axis. Symmetry-independent molecules are drawn with different colours.

full crystallographic data

IUCrData (2019). **4**, x191179 [https://doi.org/10.1107/S2414314619011799]

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Crystal data

$C_{16}H_{12}$
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Triclinic, $P\overline{1}$
a = 7.5009 (9) Å
b = 7.6819 (9) Å
c = 19.387 (3) Å
α = 99.733 (11)°
β = 100.641 (11)°
γ = 90.523 (9)°
V = 1081.2 (2) Å^3
Z = 4
$F(000)$ = 432
D_x = 1.255 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2411 reflections
θ = 2.8–28.0°
μ = 0.07 mm^{-1}
T = 193 K
Plate, colourless
0.22 × 0.15 × 0.04 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
14443 measured reflections
14443 independent reflections
7500 reflections with $I > 2\sigma(I)$
θ_{max} = 28.4°, θ_{min} = 2.7°
h = −9→9
k = −10→10
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.141
S = 1.03
14443 reflections
290 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 0.1143P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Special details

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

Refinement. Refined as a 2-component twin. BASF 0.40850 Twin law for transforming hkl(1) to hkl(2): -1.00006 0.00023 0.00003 0.00016 -1.00020 0.00001 0.95946 0.87001 1.00038
Hydrogen atoms attached to carbons were placed at calculated positions and were refined in the riding-model approximation with isotropic displacement parameters set to 1.2 U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1A	0.6265 (4)	0.1349 (3)	0.58366 (16)	0.0420 (7)
H1A	0.570270	0.239199	0.607100	0.050*
H1B	0.758394	0.160278	0.588948	0.050*
C2A	0.5377 (3)	0.0821 (3)	0.50682 (15)	0.0379 (7)
C3A	0.5094 (3)	0.1575 (3)	0.44194 (16)	0.0371 (7)
C4A	0.5622 (3)	0.3197 (3)	0.42737 (17)	0.0424 (7)
H4A	0.627703	0.406985	0.464147	0.051*
C5A	0.5171 (4)	0.3509 (4)	0.35798 (18)	0.0463 (8)
H5A	0.553328	0.460341	0.347082	0.056*
C6A	0.4206 (4)	0.2254 (4)	0.30472 (18)	0.0475 (8)
H6A	0.390593	0.250000	0.257642	0.057*
C7A	0.3663 (4)	0.0633 (4)	0.31857 (17)	0.0461 (8)
H7A	0.299603	−0.022537	0.281531	0.055*
C8A	0.4111 (3)	0.0299 (3)	0.38696 (16)	0.0396 (7)
C1B	0.9607 (4)	0.6291 (3)	0.58564 (17)	0.0485 (8)
H1C	0.834972	0.652170	0.592501	0.058*
H1D	1.040849	0.733646	0.609137	0.058*
C2B	0.9702 (4)	0.5806 (3)	0.50825 (17)	0.0428 (7)
C3B	0.9306 (3)	0.6610 (3)	0.44363 (17)	0.0416 (7)
C4B	0.8648 (4)	0.8222 (3)	0.43136 (18)	0.0472 (8)
H4B	0.837765	0.907055	0.469307	0.057*
C5B	0.8391 (4)	0.8579 (4)	0.36300 (19)	0.0512 (8)
H5B	0.792298	0.967956	0.353938	0.061*
C6B	0.8799 (4)	0.7372 (4)	0.30744 (19)	0.0523 (8)
H6B	0.862114	0.765677	0.260901	0.063*
C7B	0.9472 (4)	0.5735 (4)	0.3191 (2)	0.0537 (9)
H7B	0.974921	0.489898	0.280873	0.064*
C8B	0.9724 (3)	0.5359 (3)	0.38743 (18)	0.0439 (7)
C1C	0.6484 (4)	0.4528 (4)	0.08155 (17)	0.0491 (8)
H1E	0.760177	0.527069	0.102405	0.059*
H1F	0.670975	0.328768	0.087230	0.059*
C2C	0.5827 (3)	0.4677 (3)	0.00581 (17)	0.0422 (7)
C3C	0.6498 (4)	0.4309 (3)	−0.06130 (17)	0.0422 (7)
C4C	0.8104 (4)	0.3624 (3)	−0.07899 (18)	0.0506 (8)
H4C	0.903217	0.330126	−0.043541	0.061*
C5C	0.8316 (4)	0.3425 (3)	−0.14959 (19)	0.0530 (8)
H5C	0.939557	0.295384	−0.162728	0.064*
C6C	0.6969 (4)	0.3906 (4)	−0.20061 (19)	0.0537 (8)
H6C	0.713696	0.377195	−0.248581	0.064*
C7C	0.5370 (4)	0.4585 (4)	−0.18306 (19)	0.0512 (8)

H7C	0.445029	0.491165	−0.218706	0.061*
C8C	0.5134 (4)	0.4776 (3)	−0.11433 (17)	0.0429 (7)
C1D	0.1447 (4)	0.1273 (4)	0.08064 (18)	0.0545 (8)
H1G	0.168542	0.255730	0.083898	0.065*
H1H	0.255170	0.074407	0.103547	0.065*
C2D	0.0818 (4)	0.0383 (3)	0.00570 (18)	0.0461 (8)
C3D	0.1529 (4)	0.0084 (3)	−0.06117 (18)	0.0451 (7)
C4D	0.3153 (4)	0.0594 (3)	−0.07869 (19)	0.0525 (8)
H4D	0.406367	0.127811	−0.043834	0.063*
C5D	0.3409 (4)	0.0080 (4)	−0.1484 (2)	0.0555 (8)
H5D	0.450338	0.041999	−0.161536	0.067*
C6D	0.2082 (5)	−0.0922 (4)	−0.1985 (2)	0.0569 (9)
H6D	0.227975	−0.128483	−0.245749	0.068*
C7D	0.0464 (4)	−0.1404 (4)	−0.18077 (19)	0.0538 (8)
H7D	−0.044961	−0.208078	−0.215738	0.065*
C8D	0.0193 (4)	−0.0903 (3)	−0.11304 (19)	0.0467 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.0377 (15)	0.0378 (14)	0.0459 (19)	−0.0018 (11)	0.0034 (13)	−0.0003 (12)
C2A	0.0280 (14)	0.0375 (14)	0.046 (2)	0.0033 (11)	0.0065 (13)	0.0017 (13)
C3A	0.0260 (13)	0.0400 (14)	0.045 (2)	0.0029 (10)	0.0086 (13)	0.0063 (13)
C4A	0.0326 (14)	0.0404 (15)	0.052 (2)	−0.0012 (11)	0.0064 (14)	0.0024 (14)
C5A	0.0391 (16)	0.0437 (16)	0.059 (2)	0.0007 (12)	0.0120 (15)	0.0131 (15)
C6A	0.0438 (17)	0.0529 (17)	0.046 (2)	0.0044 (13)	0.0081 (15)	0.0107 (15)
C7A	0.0433 (17)	0.0443 (16)	0.047 (2)	0.0017 (12)	0.0047 (15)	0.0003 (14)
C8A	0.0309 (14)	0.0378 (14)	0.050 (2)	0.0030 (11)	0.0107 (14)	0.0028 (13)
C1B	0.0444 (17)	0.0417 (15)	0.058 (2)	0.0015 (12)	0.0159 (15)	−0.0037 (13)
C2B	0.0300 (13)	0.0409 (14)	0.055 (2)	−0.0026 (10)	0.0113 (13)	−0.0038 (14)
C3B	0.0285 (14)	0.0421 (15)	0.054 (2)	−0.0032 (11)	0.0119 (14)	0.0043 (14)
C4B	0.0367 (15)	0.0449 (16)	0.060 (2)	0.0036 (12)	0.0139 (15)	0.0048 (15)
C5B	0.0392 (16)	0.0478 (17)	0.068 (3)	0.0023 (12)	0.0127 (16)	0.0111 (16)
C6B	0.0483 (18)	0.0549 (18)	0.055 (2)	−0.0045 (14)	0.0114 (16)	0.0123 (16)
C7B	0.0486 (18)	0.0484 (18)	0.062 (3)	−0.0057 (14)	0.0153 (17)	−0.0023 (16)
C8B	0.0325 (14)	0.0396 (15)	0.058 (2)	−0.0045 (11)	0.0101 (14)	0.0017 (14)
C1C	0.0473 (17)	0.0473 (16)	0.051 (2)	0.0010 (13)	−0.0026 (15)	0.0165 (14)
C2C	0.0426 (15)	0.0292 (13)	0.051 (2)	−0.0031 (11)	−0.0029 (15)	0.0103 (13)
C3C	0.0506 (17)	0.0307 (14)	0.046 (2)	−0.0035 (12)	0.0108 (15)	0.0083 (13)
C4C	0.0574 (19)	0.0395 (15)	0.055 (2)	0.0042 (13)	0.0067 (17)	0.0138 (15)
C5C	0.057 (2)	0.0428 (16)	0.060 (2)	0.0033 (13)	0.0187 (18)	0.0043 (15)
C6C	0.066 (2)	0.0473 (17)	0.048 (2)	−0.0080 (15)	0.0156 (18)	0.0038 (15)
C7C	0.0547 (19)	0.0494 (17)	0.047 (2)	−0.0093 (14)	0.0039 (16)	0.0083 (15)
C8C	0.0464 (17)	0.0334 (14)	0.047 (2)	−0.0053 (12)	0.0060 (15)	0.0067 (13)
C1D	0.0495 (18)	0.0459 (16)	0.062 (2)	−0.0013 (13)	−0.0032 (16)	0.0057 (15)
C2D	0.0440 (16)	0.0286 (14)	0.059 (2)	0.0023 (11)	−0.0074 (16)	0.0065 (14)
C3D	0.0525 (18)	0.0321 (14)	0.053 (2)	0.0110 (12)	0.0115 (16)	0.0130 (13)
C4D	0.0554 (19)	0.0352 (15)	0.063 (3)	−0.0011 (13)	0.0002 (17)	0.0086 (15)

C5D	0.055 (2)	0.0489 (17)	0.069 (3)	0.0053 (14)	0.0181 (18)	0.0218 (17)
C6D	0.068 (2)	0.0544 (18)	0.051 (2)	0.0175 (16)	0.0114 (19)	0.0142 (16)
C7D	0.0508 (19)	0.0484 (17)	0.058 (2)	0.0094 (14)	−0.0006 (17)	0.0090 (16)
C8D	0.0456 (17)	0.0354 (15)	0.058 (2)	0.0071 (12)	0.0029 (16)	0.0117 (14)

Geometric parameters (Å, º)

C1A—C2A	1.500 (4)	C1C—C2C	1.484 (4)
C1A—C8A^{i}	1.518 (4)	C1C—C8C^{iii}	1.531 (4)
C1A—H1A	0.9900	C1C—H1E	0.9900
C1A—H1B	0.9900	C1C—H1F	0.9900
C2A—C2A^{i}	1.341 (4)	C2C—C2C^{iii}	1.335 (5)
C2A—C3A	1.453 (4)	C2C—C3C	1.465 (4)
C3A—C4A	1.393 (3)	C3C—C4C	1.396 (4)
C3A—C8A	1.408 (4)	C3C—C8C	1.406 (4)
C4A—C5A	1.387 (4)	C4C—C5C	1.390 (4)
C4A—H4A	0.9500	C4C—H4C	0.9500
C5A—C6A	1.376 (4)	C5C—C6C	1.377 (4)
C5A—H5A	0.9500	C5C—H5C	0.9500
C6A—C7A	1.390 (4)	C6C—C7C	1.388 (4)
C6A—H6A	0.9500	C6C—H6C	0.9500
C7A—C8A	1.374 (4)	C7C—C8C	1.360 (4)
C7A—H7A	0.9500	C7C—H7C	0.9500
C1B—C2B	1.499 (4)	C1D—C2D	1.485 (4)
C1B—C8B^{ii}	1.506 (4)	C1D—C8D^{iv}	1.526 (4)
C1B—H1C	0.9900	C1D—H1G	0.9900
C1B—H1D	0.9900	C1D—H1H	0.9900
C2B—C2B^{ii}	1.329 (5)	C2D—C2D^{iv}	1.321 (5)
C2B—C3B	1.472 (4)	C2D—C3D	1.475 (4)
C3B—C4B	1.379 (4)	C3D—C4D	1.393 (4)
C3B—C8B	1.410 (4)	C3D—C8D	1.395 (4)
C4B—C5B	1.378 (4)	C4D—C5D	1.392 (4)
C4B—H4B	0.9500	C4D—H4D	0.9500
C5B—C6B	1.379 (4)	C5D—C6D	1.380 (4)
C5B—H5B	0.9500	C5D—H5D	0.9500
C6B—C7B	1.397 (4)	C6D—C7D	1.385 (4)
C6B—H6B	0.9500	C6D—H6D	0.9500
C7B—C8B	1.384 (4)	C7D—C8D	1.357 (4)
C7B—H7B	0.9500	C7D—H7D	0.9500
C2A—C1A—C8A^{i}	101.2 (2)	C2C—C1C—C8C^{iii}	100.7 (2)
C2A—C1A—H1A	111.5	C2C—C1C—H1E	111.6
C8A^{i}—C1A—H1A	111.5	C8C^{iii}—C1C—H1E	111.6
C2A—C1A—H1B	111.5	C2C—C1C—H1F	111.6
C8A^{i}—C1A—H1B	111.5	C8C^{iii}—C1C—H1F	111.6
H1A—C1A—H1B	109.3	H1E—C1C—H1F	109.4
C2A^{i}—C2A—C3A	109.8 (3)	C2C^{iii}—C2C—C3C	109.6 (3)
C2A^{i}—C2A—C1A	111.8 (3)	C2C^{iii}—C2C—C1C	113.0 (4)

C3A—C2A—C1A	138.4 (2)	C3C—C2C—C1C	137.4 (2)
C4A—C3A—C8A	120.1 (3)	C4C—C3C—C8C	120.1 (3)
C4A—C3A—C2A	132.5 (3)	C4C—C3C—C2C	133.1 (3)
C8A—C3A—C2A	107.5 (2)	C8C—C3C—C2C	106.8 (2)
C5A—C4A—C3A	118.5 (3)	C5C—C4C—C3C	118.6 (3)
C5A—C4A—H4A	120.7	C5C—C4C—H4C	120.7
C3A—C4A—H4A	120.7	C3C—C4C—H4C	120.7
C6A—C5A—C4A	120.9 (3)	C6C—C5C—C4C	120.4 (3)
C6A—C5A—H5A	119.6	C6C—C5C—H5C	119.8
C4A—C5A—H5A	119.6	C4C—C5C—H5C	119.8
C5A—C6A—C7A	121.2 (3)	C5C—C6C—C7C	121.1 (3)
C5A—C6A—H6A	119.4	C5C—C6C—H6C	119.5
C7A—C6A—H6A	119.4	C7C—C6C—H6C	119.5
C8A—C7A—C6A	118.6 (3)	C8C—C7C—C6C	119.3 (3)
C8A—C7A—H7A	120.7	C8C—C7C—H7C	120.3
C6A—C7A—H7A	120.7	C6C—C7C—H7C	120.3
C7A—C8A—C3A	120.7 (3)	C7C—C8C—C3C	120.5 (3)
C7A—C8A—C1A^{i}	129.7 (3)	C7C—C8C—C1C^{iii}	129.5 (3)
C3A—C8A—C1A^{i}	109.6 (3)	C3C—C8C—C1C^{iii}	109.9 (3)
C2B—C1B—C8B^{ii}	101.0 (2)	C2D—C1D—C8D^{iv}	100.7 (2)
C2B—C1B—H1C	111.6	C2D—C1D—H1G	111.6
C8B^{ii}—C1B—H1C	111.6	C8D^{iv}—C1D—H1G	111.6
C2B—C1B—H1D	111.6	C2D—C1D—H1H	111.6
C8B^{ii}—C1B—H1D	111.6	C8D^{iv}—C1D—H1H	111.6
H1C—C1B—H1D	109.4	H1G—C1D—H1H	109.4
C2B^{ii}—C2B—C3B	109.3 (4)	C2D^{iv}—C2D—C3D	109.2 (4)
C2B^{ii}—C2B—C1B	112.7 (4)	C2D^{iv}—C2D—C1D	113.2 (4)
C3B—C2B—C1B	138.0 (2)	C3D—C2D—C1D	137.5 (2)
C4B—C3B—C8B	120.6 (3)	C4D—C3D—C8D	120.2 (3)
C4B—C3B—C2B	132.7 (3)	C4D—C3D—C2D	132.9 (3)
C8B—C3B—C2B	106.7 (2)	C8D—C3D—C2D	106.9 (3)
C5B—C4B—C3B	118.7 (3)	C5D—C4D—C3D	118.5 (3)
C5B—C4B—H4B	120.7	C5D—C4D—H4D	120.8
C3B—C4B—H4B	120.7	C3D—C4D—H4D	120.8
C4B—C5B—C6B	121.5 (3)	C6D—C5D—C4D	120.3 (3)
C4B—C5B—H5B	119.3	C6D—C5D—H5D	119.8
C6B—C5B—H5B	119.3	C4D—C5D—H5D	119.8
C5B—C6B—C7B	120.5 (3)	C5D—C6D—C7D	120.7 (3)
C5B—C6B—H6B	119.7	C5D—C6D—H6D	119.6
C7B—C6B—H6B	119.7	C7D—C6D—H6D	119.6
C8B—C7B—C6B	118.5 (3)	C8D—C7D—C6D	119.6 (3)
C8B—C7B—H7B	120.7	C8D—C7D—H7D	120.2
C6B—C7B—H7B	120.7	C6D—C7D—H7D	120.2
C7B—C8B—C3B	120.2 (3)	C7D—C8D—C3D	120.7 (3)
C7B—C8B—C1B^{ii}	129.5 (3)	C7D—C8D—C1D^{iv}	129.4 (3)
C3B—C8B—C1B^{ii}	110.3 (3)	C3D—C8D—C1D^{iv}	109.9 (3)
C8A^{i}—C1A—C2A—C2A^{i}	−0.1 (3)	C8C^{iii}—C1C—C2C—C2C^{iii}	0.0 (4)

C8A^{i}—C1A—C2A—C3A	−179.9 (3)	C8C^{iii}—C1C—C2C—C3C	−180.0 (3)
C2A^{i}—C2A—C3A—C4A	−178.8 (3)	C2C^{iii}—C2C—C3C—C4C	−179.4 (3)
C1A—C2A—C3A—C4A	1.0 (5)	C1C—C2C—C3C—C4C	0.6 (5)
C2A^{i}—C2A—C3A—C8A	0.1 (3)	C2C^{iii}—C2C—C3C—C8C	0.0 (3)
C1A—C2A—C3A—C8A	179.9 (3)	C1C—C2C—C3C—C8C	−180.0 (3)
C8A—C3A—C4A—C5A	−0.5 (4)	C8C—C3C—C4C—C5C	0.2 (4)
C2A—C3A—C4A—C5A	178.3 (3)	C2C—C3C—C4C—C5C	179.5 (3)
C3A—C4A—C5A—C6A	0.7 (4)	C3C—C4C—C5C—C6C	0.4 (4)
C4A—C5A—C6A—C7A	−0.4 (4)	C4C—C5C—C6C—C7C	−0.5 (4)
C5A—C6A—C7A—C8A	−0.1 (4)	C5C—C6C—C7C—C8C	0.0 (4)
C6A—C7A—C8A—C3A	0.3 (4)	C6C—C7C—C8C—C3C	0.6 (4)
C6A—C7A—C8A—C1A^{i}	−178.5 (2)	C6C—C7C—C8C—C1C^{iii}	−179.6 (2)
C4A—C3A—C8A—C7A	0.0 (4)	C4C—C3C—C8C—C7C	−0.7 (4)
C2A—C3A—C8A—C7A	−179.1 (2)	C2C—C3C—C8C—C7C	179.8 (2)
C4A—C3A—C8A—C1A^{i}	179.0 (2)	C4C—C3C—C8C—C1C^{iii}	179.5 (2)
C2A—C3A—C8A—C1A^{i}	−0.1 (3)	C2C—C3C—C8C—C1C^{iii}	0.0 (3)
C8B^{ii}—C1B—C2B—C2B^{ii}	0.2 (4)	C8D^{iv}—C1D—C2D—C2D^{iv}	−0.7 (4)
C8B^{ii}—C1B—C2B—C3B	179.7 (3)	C8D^{iv}—C1D—C2D—C3D	−179.7 (3)
C2B^{ii}—C2B—C3B—C4B	179.1 (3)	C2D^{iv}—C2D—C3D—C4D	179.8 (3)
C1B—C2B—C3B—C4B	−0.4 (5)	C1D—C2D—C3D—C4D	−1.2 (5)
C2B^{ii}—C2B—C3B—C8B	−0.4 (4)	C2D^{iv}—C2D—C3D—C8D	0.4 (4)
C1B—C2B—C3B—C8B	−179.9 (3)	C1D—C2D—C3D—C8D	179.4 (3)
C8B—C3B—C4B—C5B	0.6 (4)	C8D—C3D—C4D—C5D	−0.8 (4)
C2B—C3B—C4B—C5B	−178.9 (3)	C2D—C3D—C4D—C5D	179.9 (3)
C3B—C4B—C5B—C6B	−0.9 (4)	C3D—C4D—C5D—C6D	−0.4 (4)
C4B—C5B—C6B—C7B	0.7 (4)	C4D—C5D—C6D—C7D	1.2 (4)
C5B—C6B—C7B—C8B	−0.3 (4)	C5D—C6D—C7D—C8D	−0.8 (4)
C6B—C7B—C8B—C3B	0.0 (4)	C6D—C7D—C8D—C3D	−0.3 (4)
C6B—C7B—C8B—C1B^{ii}	178.9 (3)	C6D—C7D—C8D—C1D^{iv}	−179.6 (3)
C4B—C3B—C8B—C7B	−0.2 (4)	C4D—C3D—C8D—C7D	1.1 (4)
C2B—C3B—C8B—C7B	179.4 (2)	C2D—C3D—C8D—C7D	−179.4 (2)
C4B—C3B—C8B—C1B^{ii}	−179.3 (2)	C4D—C3D—C8D—C1D^{iv}	−179.5 (2)
C2B—C3B—C8B—C1B^{ii}	0.3 (3)	C2D—C3D—C8D—C1D^{iv}	0.0 (3)

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*; (iv) −*x*, −*y*, −*z*.