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Orthorhombic polymorph of (2*E*)-2-(2,3-dihydro-1*H*-inden-1-ylidene)-2,3-dihydro-1*H*-inden-1-one[1]

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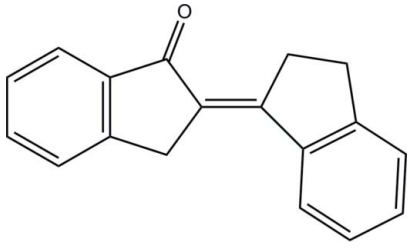
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.004 Å; R factor = 0.057; wR factor = 0.110; data-to-parameter ratio = 12.3.

The title compound, $C_{18}H_{14}O$, is polymorphic at 123 K. The orthorhombic form reported herein has two independent molecules in the asymmetric unit, with molecular volume 313.5 Å^3. The previously reported triclinic ($P\overline{1}$) form [Raston & Scott (2000). *Green Chem.*, **2**, 49–52] has molecular volume 309.6 Å^3 at the same temperature. All three molecules deviate significantly and systematically from the putative C_s symmetry ($\delta_{r.m.s.}$ = 0.0265, 0.0256, 0.0497 Å). Comparison of the two molecules in the orthorhombic polymorph shows that 16 of the 19 equivalent pairs of framework atoms have a mirror-image pattern of deviations (above/below plane), suggesting that the two are quasi-enantiomorphs. The pattern of deviations in the triclinic form is nearly the same (13 of 19 atom pairs) as the orthorhombic form.

Related literature

For the title compound co-crystallized with 2,4-di-*tert*-butylphenol, see: Turner *et al.* (2003; CSD refcode IQAZAB). For the Cambridge Structural Database (CSD), see: Allen (2002). For the determination of an absolute structure from Bijvoet pairs, see: Hooft *et al.* (2008). For the synthesis of the title compound, see: Bell & Spanswick (1966). For *cis-trans* isomerism in the title compound, see: Williams (1967).



Experimental

Crystal data

$C_{18}H_{14}O$
M_r = 246.29
Orthorhombic, $P2_12_12_1$
a = 5.291 (2) Å
b = 17.809 (5) Å
c = 26.622 (9) Å
V = 2508.5 (15) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 123 K
0.35 × 0.12 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan *HKL SCALEPACK* (Otwinowski & Minor 1997)
T_{min} = 0.973, T_{max} = 0.996
11743 measured reflections
4236 independent reflections
3145 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.110
S = 1.05
4236 reflections
344 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Absolute structure: Flack (1983), with 1665 Bijvoet pairs
Flack parameter: 0 (2)

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *IDEAL* (Gould *et al.*, 1988) and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2149).

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[1] CAS 17563-12-1.

supporting information

Acta Cryst. (2012). E**68**, o2756 [doi:10.1107/S1600536812035994]

Orthorhombic polymorph of (2*E*)-2-(2,3-dihydro-1*H*-inden-1-ylidene)-2,3-dihydro-1*H*-inden-1-one

Hairong Li, Frank R. Fronczek and Steven F. Watkins

S1. Comment

Four pairs (**Ia**, **Ib**) of independent molecules of the title compound occupy an orthorhombic unit cell at 123 K. Thirteen non-H framework atoms of **Ia**, and sixteen atoms of **Ib**, deviate significantly from their mean planes: δ_{max} = 0.053 (3) and $\delta_{r.m.s.}$ = 0.027 Å, δ_{max} = 0.052 (3) and $\delta_{r.m.s.}$ = 0.026 Å respectively. A least-squares fit of chemically equivalent pairs of non-H atomic positions (*IDEAL*, Gould *et al.*, 1988) shows an average mis-match $\delta_{r.m.s.}$ = 0.051 Å, and also reveals a mirror-image pattern of deviations (above/below plane) for sixteen of the nineteen pairs. This suggests that **Ia** and **Ib** are quasi-enantiomorphs. Indeed, a least-squares fit of the relative atomic coordinates of **Ia** to those of **Ib** inverted through the origin give an average mis-match $\delta_{r.m.s.}$ = 0.022 Å.

The triclinic form of **I** at 123 K has been reported (Raston & Scott, 2000; CCDC refcode LOLYUG; Allen, 2002). It is also significantly non-planar with $\delta/\sigma > 3$ for sixteen framework atoms. The relative atomic positions match closely those of **Ia** ($\delta_{r.m.s.}$ = 0.051 Å) and **Ib** ($\delta_{r.m.s.}$ = 0.050 Å), and the pattern of deviations for thirteen non-H atoms is identical to equivalent atoms in **Ia**.

S2. Experimental

The synthesis is detailed by Bell & Spanswick (1966): benzyl cyanide (1.8 g.) was added to a solution of sodium (0.35 g) in ethanol (20 ml). Indan-1-one (2 g) was then added, and the mixture warmed on a steam-bath for 20 min. The product was cooled, diluted, and acidified with acetic acid. The sticky precipitate was crystallized from ethanol to yield yellow needles, m.p. 141–143°C.

S3. Refinement

The absolute configuration could not be determined by analysis of 1665 Bijvoet pairs (Flack (1983) x = 0(2), Hooft *et al.* (2008) y = 0.4 (12). All H atoms were placed in calculated positions, with C—H distances of 0.95–0.99 Å, U_{iso} = 1.2 of the attached carbon atom, and thereafter treated as riding.

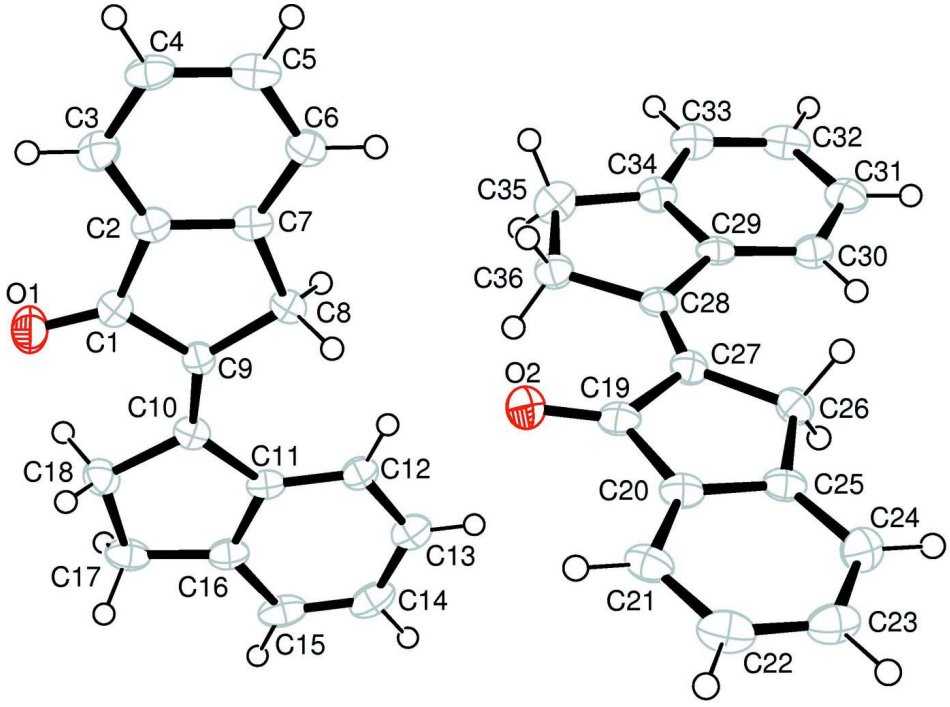

Figure 1

View of (I) (50% probability displacement ellipsoids)

(2*E*)-2-(2,3-dihydro-1*H*-inden-1-ylidene)-2,3-dihydro-1*H*- inden-1-one

Crystal data

$C_{18}H_{14}O$
$M_r = 246.29$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.291$ (2) Å
$b = 17.809$ (5) Å
$c = 26.622$ (9) Å
$V = 2508.5$ (15) Å^3
$Z = 8$
$F(000) = 1040$
$D_x = 1.304$ Mg m^{-3}
Melting point = 414–416 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2407 reflections
$\theta = 2.5$–25°
$\mu = 0.08$ mm^{-1}
$T = 123$ K
Needle, yellow
0.35 × 0.12 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: sealed tube
Horizonally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan *HKL SCALEPACK* (Otwinowski & Minor 1997)
$T_{min} = 0.973$, $T_{max} = 0.996$
11743 measured reflections
4236 independent reflections
3145 reflections with $I > 2\sigma(I)$
$R_{int} = 0.074$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.6°$
$h = -6 \rightarrow 6$
$k = -20 \rightarrow 21$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.110$
$S = 1.05$
4236 reflections
344 parameters
0 restraints
0 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2 + 1.1913P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0049 (8)
Absolute structure: Flack (1983), with 1665 Bijvoet pairs
Absolute structure parameter: 0 (2)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3862 (6)	0.10668 (16)	0.32450 (12)	0.0256 (7)
C2	0.5813 (5)	0.05703 (16)	0.30273 (11)	0.0244 (7)
C3	0.7531 (6)	0.01103 (17)	0.32733 (12)	0.0300 (8)
H3	0.7526	0.0072	0.3629	0.036*
C4	0.9248 (6)	−0.02910 (17)	0.29896 (12)	0.0309 (8)
H4	1.0456	−0.0603	0.3151	0.037*
C5	0.9216 (6)	−0.02405 (17)	0.24675 (13)	0.0310 (8)
H5	1.0391	−0.0526	0.2277	0.037*
C6	0.7499 (6)	0.02196 (16)	0.22196 (12)	0.0269 (7)
H6	0.7488	0.0252	0.1863	0.032*
C7	0.5794 (6)	0.06329 (16)	0.25077 (11)	0.0239 (8)
C8	0.3800 (5)	0.11835 (16)	0.23340 (11)	0.0238 (7)
H8A	0.2542	0.0934	0.2115	0.029*
H8B	0.4574	0.1607	0.2148	0.029*
C9	0.2586 (5)	0.14540 (16)	0.28197 (11)	0.0221 (7)
C10	0.0721 (5)	0.19601 (16)	0.28771 (11)	0.0230 (7)
C11	−0.0697 (5)	0.23669 (15)	0.24841 (11)	0.0225 (7)
C12	−0.0489 (6)	0.23430 (16)	0.19628 (11)	0.0257 (7)
H12	0.0758	0.2038	0.1807	0.031*
C13	−0.2134 (6)	0.27720 (17)	0.16749 (12)	0.0296 (8)
H13	−0.1998	0.2763	0.1319	0.036*
C14	−0.3968 (6)	0.32121 (17)	0.18995 (13)	0.0345 (9)
H14	−0.5096	0.3494	0.1696	0.041*
C15	−0.4178 (6)	0.32469 (17)	0.24150 (14)	0.0331 (8)
H15	−0.5428	0.3555	0.2567	0.04*

C16	−0.2536 (6)	0.28247 (16)	0.27084 (11)	0.0271 (8)
C17	−0.2433 (6)	0.27776 (17)	0.32697 (12)	0.0313 (8)
H17A	−0.4076	0.2609	0.3407	0.038*
H17B	−0.2005	0.3272	0.3417	0.038*
C18	−0.0346 (6)	0.21981 (18)	0.33823 (11)	0.0299 (8)
H18A	0.0994	0.2425	0.3593	0.036*
H18B	−0.1057	0.176	0.3562	0.036*
O1	0.3417 (4)	0.11400 (12)	0.36966 (8)	0.0380 (6)
C19	0.0040 (5)	−0.05063 (16)	0.07403 (12)	0.0248 (7)
C20	−0.1891 (5)	−0.09719 (15)	0.04914 (11)	0.0236 (7)
C21	−0.3649 (6)	−0.14487 (17)	0.07113 (12)	0.0293 (8)
H21	−0.3691	−0.1517	0.1065	0.035*
C22	−0.5337 (6)	−0.18215 (16)	0.04030 (13)	0.0343 (8)
H22	−0.6548	−0.2153	0.0545	0.041*
C23	−0.5264 (6)	−0.17121 (17)	−0.01129 (13)	0.0328 (8)
H23	−0.6433	−0.1973	−0.032	0.039*
C24	−0.3526 (6)	−0.12311 (16)	−0.03339 (12)	0.0301 (8)
H24	−0.3498	−0.1159	−0.0687	0.036*
C25	−0.1821 (6)	−0.08560 (16)	−0.00228 (11)	0.0237 (8)
C26	0.0229 (5)	−0.03001 (16)	−0.01635 (11)	0.0249 (7)
H26A	0.1504	−0.0535	−0.0386	0.03*
H26B	−0.0494	0.0144	−0.0335	0.03*
C27	0.1375 (5)	−0.00859 (15)	0.03373 (11)	0.0227 (7)
C28	0.3261 (5)	0.04062 (16)	0.04303 (11)	0.0224 (7)
C29	0.4744 (6)	0.08474 (16)	0.00679 (11)	0.0223 (7)
C30	0.4644 (6)	0.08748 (16)	−0.04551 (11)	0.0266 (7)
H30	0.3434	0.0585	−0.0634	0.032*
C31	0.6341 (6)	0.13329 (17)	−0.07129 (12)	0.0307 (8)
H31	0.6296	0.1352	−0.1069	0.037*
C32	0.8107 (6)	0.17629 (16)	−0.04507 (13)	0.0323 (8)
H32	0.9255	0.2072	−0.0631	0.039*
C33	0.8205 (6)	0.17441 (17)	0.00674 (13)	0.0309 (9)
H33	0.9406	0.204	0.0244	0.037*
C34	0.6521 (6)	0.12866 (16)	0.03270 (11)	0.0265 (8)
C35	0.6346 (6)	0.11740 (17)	0.08845 (11)	0.0335 (8)
H35A	0.5896	0.1649	0.1056	0.04*
H35B	0.797	0.0989	0.1022	0.04*
C36	0.4246 (6)	0.05840 (17)	0.09514 (11)	0.0284 (8)
H36A	0.4931	0.0126	0.1112	0.034*
H36B	0.2873	0.0785	0.1165	0.034*
O2	0.0410 (4)	−0.04698 (12)	0.11985 (8)	0.0332 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0271 (18)	0.0229 (17)	0.027 (2)	−0.0017 (15)	−0.0014 (14)	0.0003 (14)
C2	0.0230 (17)	0.0179 (16)	0.032 (2)	−0.0054 (15)	−0.0018 (14)	0.0011 (14)
C3	0.0305 (18)	0.0240 (18)	0.035 (2)	0.0015 (16)	−0.0022 (16)	0.0078 (15)

C4	0.0235 (17)	0.0214 (17)	0.048 (2)	0.0034 (16)	−0.0030 (16)	0.0088 (15)
C5	0.0241 (18)	0.0195 (17)	0.049 (2)	0.0000 (16)	0.0031 (16)	0.0010 (15)
C6	0.0246 (16)	0.0242 (17)	0.0318 (19)	−0.0042 (15)	0.0016 (15)	−0.0020 (15)
C7	0.0224 (17)	0.0158 (16)	0.033 (2)	−0.0026 (15)	0.0001 (15)	0.0020 (14)
C8	0.0238 (16)	0.0206 (16)	0.0269 (17)	−0.0014 (14)	0.0028 (13)	−0.0004 (13)
C9	0.0232 (16)	0.0210 (17)	0.0221 (18)	−0.0033 (15)	0.0001 (14)	−0.0006 (13)
C10	0.0237 (16)	0.0164 (16)	0.0290 (19)	−0.0032 (14)	0.0016 (14)	−0.0019 (13)
C11	0.0188 (17)	0.0147 (15)	0.034 (2)	−0.0014 (14)	−0.0013 (14)	−0.0006 (14)
C12	0.0248 (17)	0.0223 (16)	0.030 (2)	−0.0030 (15)	−0.0027 (14)	0.0000 (14)
C13	0.0284 (19)	0.0222 (17)	0.038 (2)	−0.0068 (16)	−0.0041 (15)	0.0059 (15)
C14	0.030 (2)	0.0236 (18)	0.050 (2)	−0.0043 (17)	−0.0148 (17)	0.0068 (16)
C15	0.0239 (18)	0.0188 (17)	0.057 (3)	0.0040 (15)	−0.0060 (17)	−0.0035 (16)
C16	0.0216 (16)	0.0212 (17)	0.039 (2)	−0.0073 (15)	−0.0018 (15)	−0.0019 (15)
C17	0.0240 (18)	0.0239 (18)	0.046 (2)	0.0019 (15)	0.0042 (16)	−0.0073 (15)
C18	0.0306 (18)	0.0306 (18)	0.0286 (19)	0.0003 (16)	0.0035 (14)	−0.0065 (14)
O1	0.0468 (15)	0.0413 (14)	0.0259 (14)	0.0089 (12)	0.0002 (11)	0.0016 (11)
C19	0.0214 (17)	0.0203 (17)	0.033 (2)	0.0077 (14)	−0.0001 (15)	0.0031 (14)
C20	0.0206 (17)	0.0151 (16)	0.035 (2)	0.0042 (14)	0.0008 (14)	0.0011 (14)
C21	0.0242 (17)	0.0272 (18)	0.037 (2)	0.0025 (16)	0.0068 (15)	0.0077 (15)
C22	0.0290 (19)	0.0192 (17)	0.055 (2)	−0.0037 (15)	0.0060 (17)	0.0014 (16)
C23	0.0254 (19)	0.0219 (18)	0.051 (2)	−0.0032 (16)	−0.0032 (17)	−0.0083 (16)
C24	0.033 (2)	0.0221 (17)	0.035 (2)	0.0000 (17)	−0.0015 (15)	−0.0077 (15)
C25	0.0198 (18)	0.0173 (16)	0.034 (2)	0.0037 (14)	0.0020 (13)	0.0000 (14)
C26	0.0261 (17)	0.0217 (16)	0.0268 (18)	0.0027 (15)	0.0031 (14)	−0.0007 (14)
C27	0.0230 (17)	0.0183 (16)	0.0267 (19)	0.0041 (15)	0.0018 (13)	−0.0023 (13)
C28	0.0182 (16)	0.0205 (16)	0.0286 (18)	0.0074 (15)	0.0004 (13)	−0.0011 (14)
C29	0.0178 (17)	0.0165 (16)	0.033 (2)	0.0044 (14)	0.0011 (14)	−0.0009 (14)
C30	0.0228 (17)	0.0242 (17)	0.033 (2)	0.0012 (15)	−0.0012 (14)	0.0008 (14)
C31	0.0285 (18)	0.0272 (18)	0.036 (2)	0.0068 (16)	0.0029 (15)	0.0061 (15)
C32	0.0263 (19)	0.0189 (17)	0.052 (2)	0.0001 (15)	0.0062 (16)	0.0080 (15)
C33	0.029 (2)	0.0200 (18)	0.044 (2)	0.0003 (16)	0.0005 (16)	−0.0002 (15)
C34	0.0280 (18)	0.0170 (16)	0.035 (2)	0.0039 (16)	−0.0004 (14)	−0.0005 (14)
C35	0.0361 (19)	0.0253 (18)	0.039 (2)	−0.0027 (17)	−0.0050 (16)	0.0001 (15)
C36	0.0246 (18)	0.0306 (19)	0.0300 (19)	−0.0039 (15)	0.0002 (15)	−0.0012 (14)
O2	0.0327 (13)	0.0400 (14)	0.0268 (14)	−0.0005 (11)	0.0007 (10)	0.0030 (10)

Geometric parameters (Å, º)

C1—O1	1.232 (3)	C19—O2	1.237 (3)
C1—C2	1.478 (4)	C19—C20	1.473 (4)
C1—C9	1.488 (4)	C19—C27	1.487 (4)
C2—C3	1.388 (4)	C20—C25	1.385 (4)
C2—C7	1.388 (4)	C20—C21	1.389 (4)
C3—C4	1.381 (4)	C21—C22	1.383 (4)
C3—H3	0.95	C21—H21	0.95
C4—C5	1.393 (4)	C22—C23	1.388 (4)
C4—H4	0.95	C22—H22	0.95
C5—C6	1.390 (4)	C23—C24	1.388 (4)

C5—H5	0.95	C23—H23	0.95
C6—C7	1.394 (4)	C24—C25	1.395 (4)
C6—H6	0.95	C24—H24	0.95
C7—C8	1.513 (4)	C25—C26	1.516 (4)
C8—C9	1.522 (4)	C26—C27	1.514 (4)
C8—H8A	0.99	C26—H26A	0.99
C8—H8B	0.99	C26—H26B	0.99
C9—C10	1.345 (4)	C27—C28	1.351 (4)
C10—C11	1.477 (4)	C28—C29	1.471 (4)
C10—C18	1.519 (4)	C28—C36	1.515 (4)
C11—C12	1.393 (4)	C29—C30	1.394 (4)
C11—C16	1.403 (4)	C29—C34	1.404 (4)
C12—C13	1.389 (4)	C30—C31	1.394 (4)
C12—H12	0.95	C30—H30	0.95
C13—C14	1.383 (4)	C31—C32	1.395 (4)
C13—H13	0.95	C31—H31	0.95
C14—C15	1.378 (5)	C32—C33	1.381 (4)
C14—H14	0.95	C32—H32	0.95
C15—C16	1.389 (4)	C33—C34	1.391 (4)
C15—H15	0.95	C33—H33	0.95
C16—C17	1.498 (4)	C34—C35	1.501 (4)
C17—C18	1.541 (4)	C35—C36	1.540 (4)
C17—H17A	0.99	C35—H35A	0.99
C17—H17B	0.99	C35—H35B	0.99
C18—H18A	0.99	C36—H36A	0.99
C18—H18B	0.99	C36—H36B	0.99

O1—C1—C2	125.4 (3)	O2—C19—C20	125.7 (3)
O1—C1—C9	127.4 (3)	O2—C19—C27	127.6 (3)
C2—C1—C9	107.2 (2)	C20—C19—C27	106.8 (3)
C3—C2—C7	121.5 (3)	C25—C20—C21	121.7 (3)
C3—C2—C1	128.7 (3)	C25—C20—C19	110.0 (3)
C7—C2—C1	109.7 (3)	C21—C20—C19	128.2 (3)
C4—C3—C2	118.6 (3)	C22—C21—C20	118.4 (3)
C4—C3—H3	120.7	C22—C21—H21	120.8
C2—C3—H3	120.7	C20—C21—H21	120.8
C3—C4—C5	120.3 (3)	C21—C22—C23	120.2 (3)
C3—C4—H4	119.9	C21—C22—H22	119.9
C5—C4—H4	119.9	C23—C22—H22	119.9
C6—C5—C4	121.3 (3)	C22—C23—C24	121.6 (3)
C6—C5—H5	119.3	C22—C23—H23	119.2
C4—C5—H5	119.3	C24—C23—H23	119.2
C5—C6—C7	118.2 (3)	C23—C24—C25	118.2 (3)
C5—C6—H6	120.9	C23—C24—H24	120.9
C7—C6—H6	120.9	C25—C24—H24	120.9
C2—C7—C6	120.1 (3)	C20—C25—C24	119.9 (3)
C2—C7—C8	111.2 (3)	C20—C25—C26	111.1 (3)
C6—C7—C8	128.7 (3)	C24—C25—C26	129.0 (3)

C7—C8—C9	103.9 (2)	C27—C26—C25	103.5 (2)
C7—C8—H8A	111	C27—C26—H26A	111.1
C9—C8—H8A	111	C25—C26—H26A	111.1
C7—C8—H8B	111	C27—C26—H26B	111.1
C9—C8—H8B	111	C25—C26—H26B	111.1
H8A—C8—H8B	109	H26A—C26—H26B	109
C10—C9—C1	123.9 (3)	C28—C27—C19	123.0 (3)
C10—C9—C8	128.2 (3)	C28—C27—C26	128.4 (3)
C1—C9—C8	107.9 (2)	C19—C27—C26	108.6 (2)
C9—C10—C11	128.4 (3)	C27—C28—C29	128.3 (3)
C9—C10—C18	124.1 (3)	C27—C28—C36	123.9 (3)
C11—C10—C18	107.6 (2)	C29—C28—C36	107.8 (2)
C12—C11—C16	119.8 (3)	C30—C29—C34	119.8 (3)
C12—C11—C10	130.6 (3)	C30—C29—C28	130.8 (3)
C16—C11—C10	109.6 (3)	C34—C29—C28	109.4 (3)
C13—C12—C11	118.9 (3)	C31—C30—C29	119.2 (3)
C13—C12—H12	120.5	C31—C30—H30	120.4
C11—C12—H12	120.5	C29—C30—H30	120.4
C14—C13—C12	120.8 (3)	C30—C31—C32	120.4 (3)
C14—C13—H13	119.6	C30—C31—H31	119.8
C12—C13—H13	119.6	C32—C31—H31	119.8
C15—C14—C13	120.8 (3)	C33—C32—C31	120.8 (3)
C15—C14—H14	119.6	C33—C32—H32	119.6
C13—C14—H14	119.6	C31—C32—H32	119.6
C14—C15—C16	119.0 (3)	C32—C33—C34	119.1 (3)
C14—C15—H15	120.5	C32—C33—H33	120.5
C16—C15—H15	120.5	C34—C33—H33	120.5
C15—C16—C11	120.6 (3)	C33—C34—C29	120.7 (3)
C15—C16—C17	127.9 (3)	C33—C34—C35	127.5 (3)
C11—C16—C17	111.5 (3)	C29—C34—C35	111.7 (3)
C16—C17—C18	104.9 (2)	C34—C35—C36	104.5 (2)
C16—C17—H17A	110.8	C34—C35—H35A	110.9
C18—C17—H17A	110.8	C36—C35—H35A	110.9
C16—C17—H17B	110.8	C34—C35—H35B	110.9
C18—C17—H17B	110.8	C36—C35—H35B	110.9
H17A—C17—H17B	108.8	H35A—C35—H35B	108.9
C10—C18—C17	106.3 (2)	C28—C36—C35	106.6 (2)
C10—C18—H18A	110.5	C28—C36—H36A	110.4
C17—C18—H18A	110.5	C35—C36—H36A	110.4
C10—C18—H18B	110.5	C28—C36—H36B	110.4
C17—C18—H18B	110.5	C35—C36—H36B	110.4
H18A—C18—H18B	108.7	H36A—C36—H36B	108.6
O1—C1—C2—C3	−1.5 (5)	O2—C19—C20—C25	178.1 (3)
C9—C1—C2—C3	178.2 (3)	C27—C19—C20—C25	−0.6 (3)
O1—C1—C2—C7	−179.7 (3)	O2—C19—C20—C21	0.3 (5)
C9—C1—C2—C7	0.0 (3)	C27—C19—C20—C21	−178.3 (3)
C7—C2—C3—C4	0.0 (5)	C25—C20—C21—C22	1.0 (4)

C1—C2—C3—C4	−178.0 (3)	C19—C20—C21—C22	178.5 (3)
C2—C3—C4—C5	−1.0 (5)	C20—C21—C22—C23	−0.5 (4)
C3—C4—C5—C6	1.0 (5)	C21—C22—C23—C24	−0.1 (5)
C4—C5—C6—C7	0.0 (4)	C22—C23—C24—C25	0.2 (5)
C3—C2—C7—C6	1.0 (4)	C21—C20—C25—C24	−0.9 (4)
C1—C2—C7—C6	179.4 (2)	C19—C20—C25—C24	−178.8 (2)
C3—C2—C7—C8	−178.4 (3)	C21—C20—C25—C26	178.8 (3)
C1—C2—C7—C8	0.0 (3)	C19—C20—C25—C26	0.8 (3)
C5—C6—C7—C2	−1.0 (4)	C23—C24—C25—C20	0.3 (4)
C5—C6—C7—C8	178.3 (3)	C23—C24—C25—C26	−179.3 (3)
C2—C7—C8—C9	0.0 (3)	C20—C25—C26—C27	−0.7 (3)
C6—C7—C8—C9	−179.3 (3)	C24—C25—C26—C27	178.9 (3)
O1—C1—C9—C10	0.7 (5)	O2—C19—C27—C28	0.6 (5)
C2—C1—C9—C10	−179.0 (3)	C20—C19—C27—C28	179.2 (3)
O1—C1—C9—C8	179.7 (3)	O2—C19—C27—C26	−178.5 (3)
C2—C1—C9—C8	0.0 (3)	C20—C19—C27—C26	0.1 (3)
C7—C8—C9—C10	178.9 (3)	C25—C26—C27—C28	−178.7 (3)
C7—C8—C9—C1	0.0 (3)	C25—C26—C27—C19	0.4 (3)
C1—C9—C10—C11	−179.0 (3)	C19—C27—C28—C29	179.2 (3)
C8—C9—C10—C11	2.3 (5)	C26—C27—C28—C29	−1.9 (5)
C1—C9—C10—C18	−0.6 (4)	C19—C27—C28—C36	0.4 (4)
C8—C9—C10—C18	−179.4 (3)	C26—C27—C28—C36	179.4 (3)
C9—C10—C11—C12	−0.5 (5)	C27—C28—C29—C30	−0.8 (5)
C18—C10—C11—C12	−179.0 (3)	C36—C28—C29—C30	178.1 (3)
C9—C10—C11—C16	178.1 (3)	C27—C28—C29—C34	−179.8 (3)
C18—C10—C11—C16	−0.4 (3)	C36—C28—C29—C34	−0.9 (3)
C16—C11—C12—C13	−0.5 (4)	C34—C29—C30—C31	0.8 (4)
C10—C11—C12—C13	178.0 (3)	C28—C29—C30—C31	−178.1 (3)
C11—C12—C13—C14	−0.5 (4)	C29—C30—C31—C32	−0.5 (4)
C12—C13—C14—C15	1.2 (5)	C30—C31—C32—C33	−0.1 (5)
C13—C14—C15—C16	−0.8 (5)	C31—C32—C33—C34	0.3 (5)
C14—C15—C16—C11	−0.3 (5)	C32—C33—C34—C29	0.1 (4)
C14—C15—C16—C17	−179.9 (3)	C32—C33—C34—C35	178.7 (3)
C12—C11—C16—C15	0.9 (4)	C30—C29—C34—C33	−0.7 (4)
C10—C11—C16—C15	−177.9 (3)	C28—C29—C34—C33	178.5 (3)
C12—C11—C16—C17	−179.4 (3)	C30—C29—C34—C35	−179.5 (3)
C10—C11—C16—C17	1.8 (3)	C28—C29—C34—C35	−0.3 (3)
C15—C16—C17—C18	177.2 (3)	C33—C34—C35—C36	−177.3 (3)
C11—C16—C17—C18	−2.4 (3)	C29—C34—C35—C36	1.4 (3)
C9—C10—C18—C17	−179.7 (3)	C27—C28—C36—C35	−179.3 (3)
C11—C10—C18—C17	−1.0 (3)	C29—C28—C36—C35	1.7 (3)
C16—C17—C18—C10	2.0 (3)	C34—C35—C36—C28	−1.8 (3)