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ISSN 2414-3146

2,3-Dihydro-1*H*-cyclopenta[*b*]naphthalene-4,9-dione

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Received 2 December 2020
Accepted 11 February 2021

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

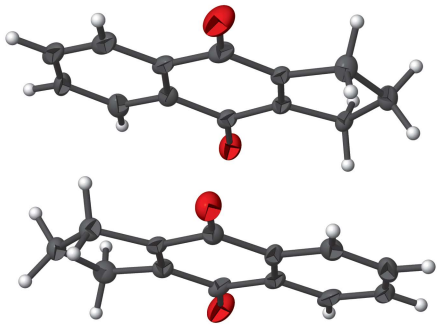
Keywords: naphthoquinone; retro Diels–Alder reaction; cycloreversion; planarity; crystal structure.

CCDC reference: 2046748

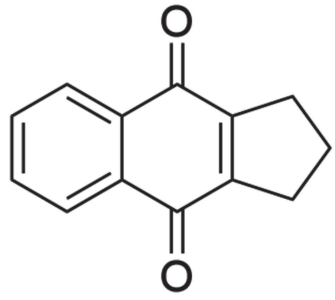
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{13}H_{10}O_2$, crystallizes with two almost planar molecules in the asymmetric unit. In the crystal, slipped π–π stacking interactions help to establish the packing with the shortest centroid–centroid separation being 3.8195 (18) Å.

3D view



Chemical scheme



Structure description

Several kinds of naphthoquinone ring-containing compounds have been encountered in nature that are known to be biologically important molecules (Qiu *et al.*, 2018). Naphthoquinones are also important constituents of a variety of quinone-based dyes upon ring fusion with heterocyclic system (Katritzky *et al.*, 1988). We now describe the synthesis and structure of the title compound, **2**.

Compound **2** crystallizes with two almost planar molecules in the asymmetric unit (Fig. 1). For the C1-molecule, the C═O bonds (C1═O1 and C8═O2) are almost the same length [1.221 (4) Å and 1.225 (4) Å, respectively]. The C9═C13 double bond connected with the fused cyclopentane ring is shorter [1.343 (5) Å] than the equivalent bond found in 2-hydroxy-3-(2-methylprop-1-en-1-yl)naphthalene 1,4-dione (Alcantara Emiliano *et al.*, 2016; Cambridge Structural Database refcode XAHPAA) [1.361 (3) Å] due, presumably, to ring strain (Fig. 1). A difference of 2° is found between the angles C1—C13—C9 [123.2 (3)°] and C8—C9—C13 [121.7 (3)°] in the title compound whereas in XAHPAA this difference is about 4° owing to the different substituents. The second C14 molecule, with a similar geometry to the C1 molecule, completes the asymmetric unit of the title compound.

The packing is represented in Fig. 2. There is no direct evidence of any intra- or intermolecular hydrogen bonding in the system. Adjacent molecules are stacked in an angular (shifted) orientation and several slipped aromatic π–π stacking interactions help

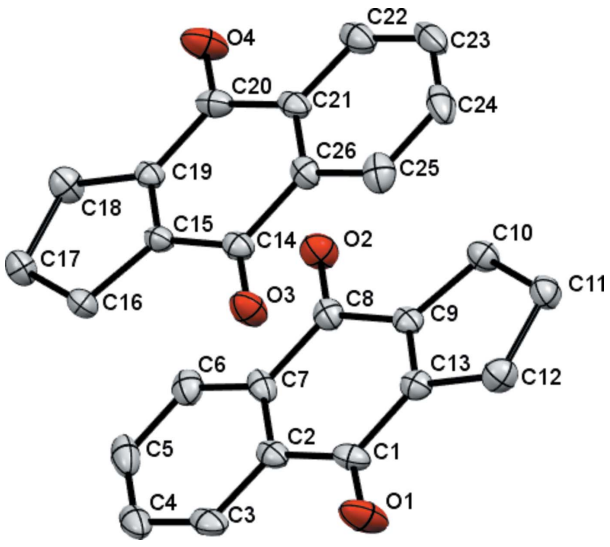


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% level while H atoms are omitted for clarity.

to establish the packing, the shortest centroid–centroid separation being 3.8195 (18) Å (slippage = 1.722 Å) for the C1/C2/C7–C9/C13 and C14/C15/C19–C21/C26 rings.

Synthesis and crystallization

As part of our studies of Diels–Alder chemistry, we explored the DA reaction between 1,3-cyclohexadiene and the quinone derivative **1** at 170°C in a sealed tube for 12 h (Fig. 3). To our surprise, instead of forming the expected DA adduct **3**, the aromatized title compound was achieved in an excellent yield (86%) as a yellow crystalline solid. We suggest that initially the expected [4 + 2] cycloaddition reaction happened, but at high temperature the cycloadduct underwent cycloreversion (retro-DA reaction), resulting in the elimination of a volatile ethylene molecule and aromatization. The compound was recrystallized from mixed solvents of petroleum ether and ethyl acetate (4:1) in the refrigerator. Yellow crystalline solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.06 (*J* = 5.72, 3.37 Hz, 2H), 7.70 (*dd*, *J* = 5.65, 3.31 Hz, 2H), 2.94 (*t*, *J* = 7.75 Hz, 4H), 2.09 (*m*, 2H) p.p.m.; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 183.9, 151.2, 133.3, 133.1, 126.1, 31.1, 21.5 p.p.m.. (Clausen *et al.*, 2001; Franck *et al.*, 1985).

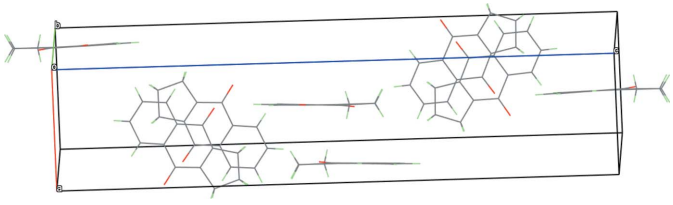


Figure 2
The crystal packing viewed along the *b*-axis direction.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{10}O_2$
M_r	198.22
Crystal system, space group	Tetragonal, $P4_3$
Temperature (K)	150
a, *c* (Å)	7.4781 (1), 33.0219 (10)
V (Å^3)	1846.65 (7)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	0.10
Crystal size (mm)	0.21 × 0.13 × 0.04
Data collection	
Diffractometer	Rigaku Oxford Diffraction CCD
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018)
T_{min}, T_{max}	0.636, 1.000
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	46308, 3230, 2851
R_{int}	0.150
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.060, 0.182, 1.05
No. of reflections	3230
No. of parameters	271
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.32
Absolute structure	Flack (1983)
Absolute structure parameter	1.0 (16)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *olex2.solve* (Bourhis *et al.*, 2015), *olex2.refine* (Bourhis *et al.*, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

We thank Mr Darshan S Mhatre for his help in collecting the X-ray data and with the structure refinement.

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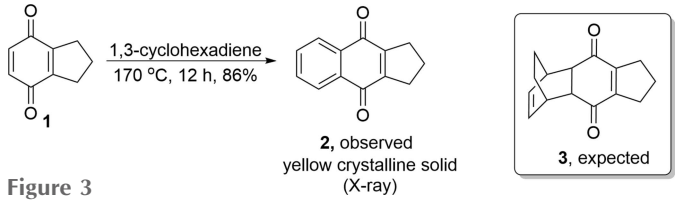

Figure 3
Synthesis scheme for the title compound.

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full crystallographic data

IUCrData (2021). **6**, x210167 [https://doi.org/10.1107/S241431462100167X]

2,3-Dihydro-1*H*-cyclopenta[*b*]naphthalene-4,9-dione

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2,3-Dihydro-1*H*-cyclopenta[*b*]naphthalene-4,9-dione

Crystal data

$C_{13}H_{10}O_2$
M_r = 198.22
Tetragonal, $P4_3$
a = 7.4781 (1) Å
c = 33.0219 (10) Å
V = 1846.65 (7) Å^3
Z = 8
F(000) = 832.447
D_x = 1.426 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 16230 reflections
θ = 2.5–30.9°
μ = 0.10 mm^{-1}
T = 150 K
Block, colourless
0.21 × 0.13 × 0.04 mm

Data collection

Rigaku Oxford Diffraction CCD diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2018)
T_{min} = 0.636, T_{max} = 1.000
46308 measured reflections
3230 independent reflections
2851 reflections with $I \geq 2u(I)$
R_{int} = 0.150
θ_{max} = 25.0°, θ_{min} = 2.5°
h = −10→10
k = −10→10
l = −46→47

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.182
S = 1.05
3230 reflections
271 parameters
1 restraint
34 constraints
Primary atom site location: iterative
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1209P)^2 + 0.4577P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.0002
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 1.0 (16)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	−0.1998 (3)	−1.0652 (3)	−0.53158 (8)	0.0313 (6)
O3	−0.4644 (3)	−0.5372 (3)	−0.46901 (7)	0.0314 (6)
O1	0.0178 (4)	−0.5172 (4)	−0.43869 (8)	0.0414 (7)
O4	−0.6811 (4)	−1.0853 (4)	−0.56192 (8)	0.0395 (7)
C13	−0.0343 (4)	−0.6351 (4)	−0.50334 (11)	0.0217 (8)

C8	−0.1458 (4)	−0.9450 (4)	−0.50952 (11)	0.0223 (8)
C15	−0.5855 (4)	−0.8269 (5)	−0.47358 (9)	0.0199 (7)
C7	−0.1437 (4)	−0.9603 (4)	−0.46489 (11)	0.0233 (8)
C2	−0.0910 (4)	−0.8149 (5)	−0.44071 (10)	0.0229 (8)
C1	−0.0324 (4)	−0.6440 (4)	−0.45901 (11)	0.0239 (8)
C16	−0.5999 (4)	−0.8685 (4)	−0.42918 (9)	0.0232 (7)
H16a	−0.4821 (4)	−0.8576 (4)	−0.41571 (9)	0.0278 (9)*
H16b	−0.6857 (4)	−0.7871 (4)	−0.41571 (9)	0.0278 (9)*
C6	−0.1933 (5)	−1.1217 (5)	−0.44638 (11)	0.0276 (8)
H6	−0.2294 (5)	−1.2205 (5)	−0.46249 (11)	0.0331 (10)*
C9	−0.0811 (4)	−0.7738 (4)	−0.52694 (9)	0.0202 (7)
C26	−0.5235 (4)	−0.6405 (4)	−0.53587 (11)	0.0218 (8)
C18	−0.6846 (5)	−1.1272 (5)	−0.47248 (10)	0.0272 (8)
H18a	−0.6030 (5)	−1.2287 (5)	−0.47791 (10)	0.0327 (10)*
H18b	−0.8087 (5)	−1.1644 (5)	−0.47857 (10)	0.0327 (10)*
C17	−0.6672 (5)	−1.0628 (4)	−0.42807 (10)	0.0257 (8)
H17a	−0.5815 (5)	−1.1392 (4)	−0.41314 (10)	0.0308 (9)*
H17b	−0.7846 (5)	−1.0690 (4)	−0.41429 (10)	0.0308 (9)*
C14	−0.5197 (4)	−0.6577 (4)	−0.49071 (10)	0.0219 (7)
C20	−0.6329 (4)	−0.9584 (4)	−0.54108 (11)	0.0260 (8)
C10	−0.0680 (4)	−0.7337 (4)	−0.57106 (10)	0.0240 (7)
H10a	0.0172 (4)	−0.8154 (4)	−0.58461 (10)	0.0288 (9)*
H10b	−0.1862 (4)	−0.7440 (4)	−0.58437 (10)	0.0288 (9)*
C21	−0.5758 (4)	−0.7871 (5)	−0.56003 (10)	0.0242 (8)
C25	−0.4721 (5)	−0.4794 (5)	−0.55371 (12)	0.0293 (8)
H25	−0.4349 (5)	−0.3815 (5)	−0.53744 (12)	0.0352 (10)*
C4	−0.1399 (4)	−0.9941 (6)	−0.38067 (12)	0.0334 (9)
H4	−0.1397 (4)	−1.0054 (6)	−0.35201 (12)	0.0401 (11)*
C24	−0.4762 (5)	−0.4644 (5)	−0.59580 (11)	0.0337 (9)
H24	−0.4440 (5)	−0.3544 (5)	−0.60823 (11)	0.0404 (11)*
C19	−0.6330 (4)	−0.9670 (4)	−0.49681 (11)	0.0197 (8)
C11	0.0008 (5)	−0.5378 (4)	−0.57204 (10)	0.0265 (8)
H11a	0.1181 (5)	−0.5317 (4)	−0.58585 (10)	0.0318 (9)*
H11b	−0.0847 (5)	−0.4605 (4)	−0.58681 (10)	0.0318 (9)*
C12	0.0185 (5)	−0.4755 (5)	−0.52765 (11)	0.0282 (8)
H12a	−0.0620 (5)	−0.3733 (5)	−0.52209 (11)	0.0339 (10)*
H12b	0.1430 (5)	−0.4396 (5)	−0.52153 (11)	0.0339 (10)*
C22	−0.5754 (5)	−0.7690 (5)	−0.60195 (10)	0.0306 (8)
H22	−0.6086 (5)	−0.8673 (5)	−0.61857 (10)	0.0368 (10)*
C23	−0.5266 (4)	−0.6074 (6)	−0.61955 (11)	0.0350 (9)
H23	−0.5279 (4)	−0.5954 (6)	−0.64819 (11)	0.0420 (11)*
C3	−0.0899 (4)	−0.8328 (5)	−0.39846 (10)	0.0292 (8)
H3	−0.0550 (4)	−0.7348 (5)	−0.38194 (10)	0.0351 (10)*
C5	−0.1894 (5)	−1.1370 (5)	−0.40428 (11)	0.0342 (9)
H5	−0.2213 (5)	−1.2470 (5)	−0.39185 (11)	0.0410 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0404 (14)	0.0252 (13)	0.0283 (13)	−0.0019 (11)	−0.0009 (11)	−0.0025 (10)
O3	0.0432 (15)	0.0280 (13)	0.0231 (13)	−0.0011 (11)	−0.0008 (11)	−0.0038 (11)
O1	0.0612 (18)	0.0350 (15)	0.0278 (15)	−0.0011 (12)	−0.0138 (13)	−0.0077 (13)
O4	0.0519 (17)	0.0388 (15)	0.0278 (14)	0.0009 (12)	−0.0114 (12)	−0.0089 (12)
C13	0.0200 (17)	0.0225 (19)	0.0226 (19)	0.0046 (13)	−0.0004 (12)	−0.0008 (12)
C8	0.0207 (16)	0.0237 (17)	0.0224 (18)	0.0048 (13)	0.0017 (13)	0.0018 (14)
C15	0.0193 (16)	0.0252 (17)	0.0152 (17)	0.0025 (13)	−0.0011 (13)	−0.0021 (13)
C7	0.0214 (18)	0.0285 (19)	0.0201 (18)	0.0087 (14)	0.0030 (12)	0.0069 (13)
C2	0.0180 (16)	0.0321 (19)	0.0186 (17)	0.0082 (13)	−0.0012 (13)	0.0000 (14)
C1	0.0257 (19)	0.0261 (19)	0.0198 (18)	0.0070 (14)	−0.0066 (12)	−0.0026 (13)
C16	0.0254 (17)	0.0268 (18)	0.0172 (17)	−0.0004 (13)	−0.0023 (14)	0.0036 (14)
C6	0.0210 (17)	0.032 (2)	0.0299 (19)	0.0049 (13)	0.0032 (14)	0.0059 (16)
C9	0.0165 (15)	0.0245 (17)	0.0198 (18)	0.0058 (12)	−0.0016 (12)	0.0016 (13)
C26	0.0207 (17)	0.0245 (18)	0.0202 (19)	0.0072 (13)	0.0032 (12)	−0.0001 (13)
C18	0.036 (2)	0.0204 (17)	0.0253 (19)	0.0014 (13)	0.0009 (15)	−0.0004 (14)
C17	0.0302 (18)	0.0264 (18)	0.0205 (17)	0.0016 (14)	0.0034 (14)	0.0011 (14)
C14	0.0215 (16)	0.0242 (17)	0.0200 (18)	0.0042 (13)	−0.0013 (12)	0.0002 (14)
C20	0.0250 (19)	0.031 (2)	0.022 (2)	0.0047 (14)	−0.0052 (13)	−0.0060 (14)
C10	0.0271 (18)	0.0243 (17)	0.0207 (17)	0.0020 (13)	0.0008 (14)	−0.0027 (14)
C21	0.0188 (17)	0.036 (2)	0.0173 (16)	0.0076 (14)	−0.0020 (13)	−0.0008 (14)
C25	0.0279 (19)	0.0276 (19)	0.032 (2)	0.0069 (14)	0.0060 (15)	0.0049 (16)
C4	0.0206 (18)	0.056 (2)	0.0234 (19)	0.0075 (15)	0.0009 (13)	0.0121 (17)
C24	0.0265 (19)	0.046 (2)	0.028 (2)	0.0086 (16)	0.0044 (15)	0.0196 (17)
C19	0.0178 (16)	0.0238 (19)	0.0176 (18)	0.0040 (13)	−0.0009 (12)	0.0010 (12)
C11	0.0280 (18)	0.0280 (18)	0.0235 (18)	0.0000 (13)	0.0009 (14)	0.0057 (15)
C12	0.0293 (18)	0.0250 (17)	0.030 (2)	−0.0005 (13)	0.0003 (15)	−0.0028 (15)
C22	0.0252 (18)	0.047 (2)	0.0198 (17)	0.0102 (15)	0.0000 (14)	−0.0021 (16)
C23	0.0242 (19)	0.064 (3)	0.0165 (18)	0.0111 (17)	0.0017 (13)	0.0057 (18)
C3	0.0209 (17)	0.044 (2)	0.0225 (18)	0.0096 (14)	−0.0060 (14)	−0.0002 (16)
C5	0.0239 (18)	0.046 (2)	0.033 (2)	0.0082 (15)	0.0094 (16)	0.0156 (18)

Geometric parameters (Å, º)

O2—C8	1.225 (4)	C18—C17	1.549 (5)
O3—C14	1.223 (4)	C18—C19	1.493 (5)
O1—C1	1.221 (4)	C17—H17a	0.9900
O4—C20	1.226 (4)	C17—H17b	0.9900
C13—C1	1.465 (5)	C20—C21	1.488 (5)
C13—C9	1.343 (5)	C20—C19	1.463 (5)
C13—C12	1.492 (5)	C10—H10a	0.9900
C8—C7	1.478 (5)	C10—H10b	0.9900
C8—C9	1.485 (5)	C10—C11	1.553 (5)
C15—C16	1.503 (4)	C21—C22	1.391 (5)
C15—C14	1.471 (5)	C25—H25	0.9500
C15—C19	1.346 (5)	C25—C24	1.395 (5)

C7—C2	1.406 (5)	C4—H4	0.9500
C7—C6	1.403 (5)	C4—C3	1.393 (5)
C2—C1	1.480 (5)	C4—C5	1.373 (6)
C2—C3	1.402 (5)	C24—H24	0.9500
C16—H16a	0.9900	C24—C23	1.379 (6)
C16—H16b	0.9900	C11—H11a	0.9900
C16—C17	1.538 (5)	C11—H11b	0.9900
C6—H6	0.9500	C11—C12	1.544 (5)
C6—C5	1.395 (5)	C12—H12a	0.9900
C9—C10	1.491 (4)	C12—H12b	0.9900
C26—C14	1.497 (5)	C22—H22	0.9500
C26—C21	1.411 (5)	C22—C23	1.390 (5)
C26—C25	1.395 (5)	C23—H23	0.9500
C18—H18a	0.9900	C3—H3	0.9500
C18—H18b	0.9900	C5—H5	0.9500

C9—C13—C1	123.2 (3)	C21—C20—O4	121.0 (3)
C12—C13—C1	124.8 (3)	C19—C20—O4	121.8 (3)
C12—C13—C9	112.0 (3)	C19—C20—C21	117.3 (3)
C7—C8—O2	122.6 (3)	H10a—C10—C9	111.08 (18)
C9—C8—O2	120.6 (3)	H10b—C10—C9	111.08 (17)
C9—C8—C7	116.7 (3)	H10b—C10—H10a	109.0
C14—C15—C16	125.2 (3)	C11—C10—C9	103.4 (3)
C19—C15—C16	112.1 (3)	C11—C10—H10a	111.08 (18)
C19—C15—C14	122.6 (3)	C11—C10—H10b	111.08 (19)
C2—C7—C8	120.6 (3)	C20—C21—C26	120.7 (3)
C6—C7—C8	119.9 (3)	C22—C21—C26	119.1 (3)
C6—C7—C2	119.5 (3)	C22—C21—C20	120.2 (3)
C1—C2—C7	121.3 (3)	H25—C25—C26	120.5 (2)
C3—C2—C7	119.5 (3)	C24—C25—C26	119.0 (4)
C3—C2—C1	119.2 (3)	C24—C25—H25	120.5 (2)
C13—C1—O1	121.1 (3)	C3—C4—H4	119.8 (2)
C2—C1—O1	122.5 (3)	C5—C4—H4	119.8 (2)
C2—C1—C13	116.3 (3)	C5—C4—C3	120.4 (4)
H16a—C16—C15	110.96 (17)	H24—C24—C25	119.7 (2)
H16b—C16—C15	110.96 (17)	C23—C24—C25	120.7 (4)
H16b—C16—H16a	109.0	C23—C24—H24	119.7 (2)
C17—C16—C15	104.0 (3)	C18—C19—C15	112.7 (3)
C17—C16—H16a	110.96 (18)	C20—C19—C15	122.3 (3)
C17—C16—H16b	110.96 (18)	C20—C19—C18	125.0 (3)
H6—C6—C7	120.0 (2)	H11a—C11—C10	110.31 (18)
C5—C6—C7	119.9 (4)	H11b—C11—C10	110.31 (19)
C5—C6—H6	120.0 (2)	H11b—C11—H11a	108.6
C8—C9—C13	121.7 (3)	C12—C11—C10	107.1 (3)
C10—C9—C13	113.3 (3)	C12—C11—H11a	110.31 (17)
C10—C9—C8	125.0 (3)	C12—C11—H11b	110.31 (18)
C21—C26—C14	120.1 (3)	C11—C12—C13	104.3 (3)
C25—C26—C14	119.3 (3)	H12a—C12—C13	110.90 (19)

C25—C26—C21	120.6 (3)	H12a—C12—C11	110.90 (18)
H18b—C18—H18a	109.0	H12b—C12—C13	110.90 (18)
C17—C18—H18a	111.00 (19)	H12b—C12—C11	110.90 (17)
C17—C18—H18b	111.00 (18)	H12b—C12—H12a	108.9
C19—C18—H18a	111.00 (18)	H22—C22—C21	120.0 (2)
C19—C18—H18b	111.00 (18)	C23—C22—C21	120.1 (4)
C19—C18—C17	103.8 (3)	C23—C22—H22	120.0 (2)
C18—C17—C16	107.4 (3)	C22—C23—C24	120.6 (4)
H17a—C17—C16	110.24 (18)	H23—C23—C24	119.7 (2)
H17a—C17—C18	110.24 (19)	H23—C23—C22	119.7 (2)
H17b—C17—C16	110.24 (19)	C4—C3—C2	120.1 (4)
H17b—C17—C18	110.24 (19)	H3—C3—C2	120.0 (2)
H17b—C17—H17a	108.5	H3—C3—C4	120.0 (2)
C15—C14—O3	121.4 (3)	C4—C5—C6	120.5 (4)
C26—C14—O3	121.8 (3)	H5—C5—C6	119.7 (2)
C26—C14—C15	116.8 (3)	H5—C5—C4	119.7 (2)

O2—C8—C7—C2	−176.0 (3)	C8—C7—C2—C3	−179.9 (3)
O2—C8—C7—C6	4.5 (4)	C8—C7—C6—C5	179.3 (3)
O2—C8—C9—C13	174.8 (3)	C8—C9—C10—C11	178.4 (3)
O2—C8—C9—C10	−2.6 (4)	C15—C16—C17—C18	1.4 (3)
O3—C14—C15—C16	2.7 (4)	C15—C14—C26—C21	−4.6 (3)
O3—C14—C15—C19	−174.3 (3)	C15—C14—C26—C25	176.5 (3)
O3—C14—C26—C21	175.3 (3)	C15—C19—C18—C17	1.7 (3)
O3—C14—C26—C25	−3.7 (4)	C15—C19—C20—C21	0.6 (3)
O1—C1—C13—C9	177.1 (3)	C7—C2—C3—C4	0.3 (3)
O1—C1—C13—C12	−1.4 (4)	C7—C6—C5—C4	1.0 (4)
O1—C1—C2—C7	−178.3 (3)	C2—C3—C4—C5	0.4 (4)
O1—C1—C2—C3	0.2 (4)	C16—C17—C18—C19	−1.8 (3)
O4—C20—C21—C26	178.9 (3)	C6—C5—C4—C3	−1.1 (4)
O4—C20—C21—C22	−0.4 (4)	C9—C10—C11—C12	−1.4 (3)
O4—C20—C19—C15	−178.0 (3)	C26—C21—C20—C19	0.3 (3)
O4—C20—C19—C18	1.9 (4)	C26—C21—C22—C23	−1.0 (3)
C13—C1—C2—C7	0.6 (3)	C26—C25—C24—C23	−1.4 (4)
C13—C1—C2—C3	179.1 (3)	C18—C19—C20—C21	−179.5 (3)
C13—C9—C8—C7	−4.4 (3)	C20—C21—C22—C23	178.3 (3)
C13—C9—C10—C11	0.8 (3)	C21—C22—C23—C24	0.7 (4)
C13—C12—C11—C10	1.5 (3)	C25—C24—C23—C22	0.5 (4)
C8—C7—C2—C1	−1.4 (3)		