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1,7,7-Trimethyl-3-(naphthalen-2-ylcarbonyl)bicyclo[2.2.1]heptan-2-one

Sabrina Bendia,[a] Kamel Ouari,[a] Mustapha Ait Ali,[b] Larbi el Firdousi[b] and Alexander Y. Nazarenko[c]*

[a]Laboratoire d'Electrochimie, d'Ingénierie Moléculaire et de Catalyse Rédox (LEIMCR), Faculté de Technologie, Université Ferhat Abbas-Sétif-1, Sétif, 19000 , Algeria, [b]Université Cadi Ayyad Faculté des Sciences Semlalia, Departement de Chimie, BP 2390, 40001, Marrakech, Morocco, and [c]Chemistry Department, State University of New York, College at Buffalo, 1300 Elmwood Ave, Buffalo, NY 14222-1095, USA. *Correspondence e-mail: nazareay@buffalostate.edu

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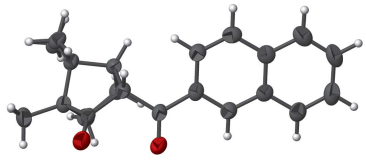
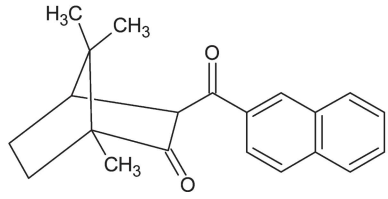
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{21}H_{22}O_2$, crystallizes in its keto form. The molecules are connected *via* weak C—H···O interactions, forming infinite chains perpendicular to the [001] axis.

3D view



Chemical scheme



Structure description

Chiral β-diketonato ligands are used in catalysis and spectroscopy; chiral naphthyl derivatives have recently been prepared (Clark *et al.*, 2013). However, no naphthyl-substituted β-diketones were found in the Cambridge Structure Database (Groom *et al.*, 2016) in November 2020.

The title compound, $C_{21}H_{22}O_2$, crystallizes in its keto-form (Fig. 1). The shape of both the camphor and naphthyl fragments is essentially the same as in their parent molecules.

There are no strong intermolecular interactions in this structure. The molecules are connected *via* weak C—H···O bonds (Table 1), forming infinite chains perpendicular to the [001] axis (Fig. 2). The hydrogen atoms of the naphthyl ring system and atoms H9*B*, H9*C*, and H10*B* of the methyl groups of the camphor fragment help to assemble these chains in the crystal *via* van der Waals interactions.

Synthesis and crystallization

The title compound was prepared by a procedure reported earlier (Clark *et al.*, 2013) and was purified by recrystallization from hexane solution (m.p. 399 K). Elemental analysis for $C_{21}H_{22}O_2$, calculated C 82.30, H 7.24; found C 82.23, H 7.15. ^{1}H NMR: (DMSO-d_6, δ p.p.m.): 12.50 (*s*, OH), 9.00–7.40 (*m*, H_{Ar}), 2.80–0.80 (*m*, $H_{Camphor}$); ^{13}C NMR: (DMSO-d_6,

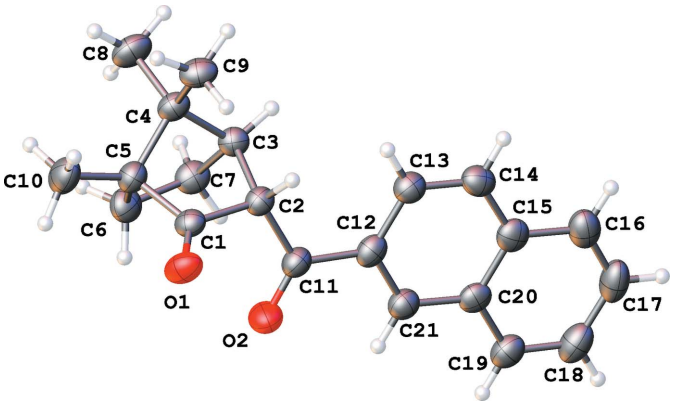


Figure 1
Numbering scheme of the title compound with 50% probability displacement ellipsoids.

δ p.p.m.): 212–194 (C═O), 135–115 (C_{Ar}), 64–9 ($C_{Camphor}$). UV–vis in acetonitrile (λ_{max} (nm), [ε] (l mol^{-1} cm^{-1}])): 272 [10197], 283 [12668], 292 [10352], 325 [8294]. Single crystals were grown by slow evaporation of a methanol solution at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

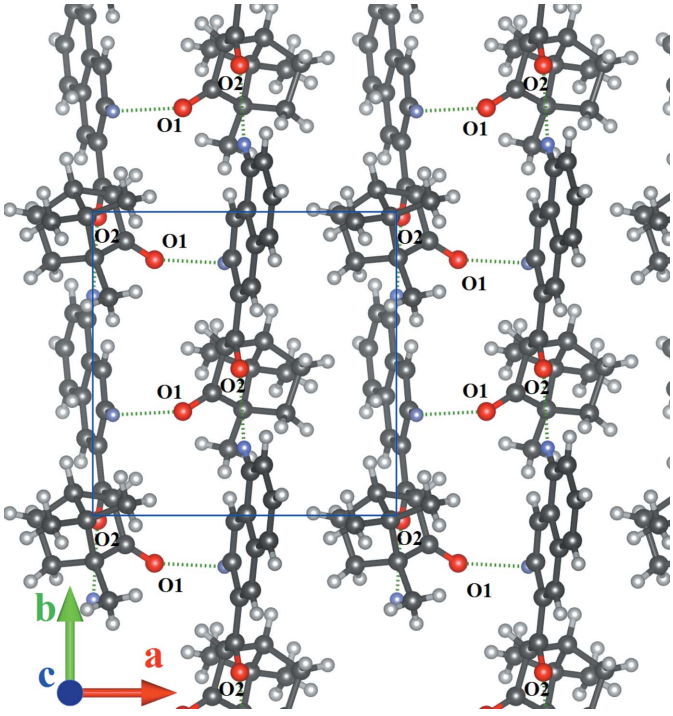


Figure 2
Packing diagram of the title compound showing C—H···O hydrogen bonding; the view along the [001] vector, which is parallel to the $\mathbf{4_1}$ screw axis. Only one layer of molecules is shown; the screw-axis symmetry operation rotates each subsequent layer by 90° and moves by $c/4$.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O1^{i}	0.95	2.57	3.296 (3)	134
C16—H16···O2^{ii}	0.95	2.57	3.458 (3)	156

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{5}{4}$; (ii) $x, y-1, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{22}O_2$
M_r	306.38
Crystal system, space group	Tetragonal, $P4_12_12$
Temperature (K)	173
a, c (Å)	9.5637 (3), 36.3395 (10)
V (Å^3)	3323.8 (2)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.60
Crystal size (mm)	0.41 × 0.33 × 0.17
Data collection	
Diffractometer	Bruker PHOTON-100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.922, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27362, 3363, 3123
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.627
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.110, 1.05
No. of reflections	3363
No. of parameters	211
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.16
Absolute structure	Flack x determined using 1176 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter	−0.04 (10)

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *VESTA* (Momma & Izumi, 2011).

Acknowledgements

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full crystallographic data

IUCrData (2020). **5**, x201662 [https://doi.org/10.1107/S2414314620016624]

1,7,7-Trimethyl-3-(naphthalen-2-ylcarbonyl)bicyclo[2.2.1]heptan-2-one

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(1*R*,3*S*,4*R*)-1,7,7-Trimethyl-3-(naphthalen-2-ylcarbonyl)bicyclo[2.2.1]heptan-2-one

Crystal data

$C_{21}H_{22}O_2$
M_r = 306.38
Tetragonal, $P4_12_12$
a = 9.5637 (3) Å
c = 36.3395 (10) Å
V = 3323.8 (2) Å^3
Z = 8
F(000) = 1312
D_x = 1.225 Mg m^{-3}
Melting point: 399 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9853 reflections
θ = 4.6–74.7°
μ = 0.60 mm^{-1}
T = 173 K
Block, colourless
0.41 × 0.33 × 0.17 mm

Data collection

Bruker PHOTON-100 CMOS diffractometer
Radiation source: sealedtube
Detector resolution: 10.8 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.922, T_{max} = 1.000
27362 measured reflections
3363 independent reflections
3123 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 75.2°, θ_{min} = 4.8°
h = −11→9
k = −11→10
l = −43→45

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.110
S = 1.05
3363 reflections
211 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 0.9139P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack x determined using 1176 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter: −0.04 (10)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.70347 (19)	0.6575 (2)	0.64361 (5)	0.0464 (4)
O2	0.5159 (2)	0.51669 (19)	0.69923 (4)	0.0496 (5)
C1	0.6066 (2)	0.5955 (2)	0.62993 (5)	0.0332 (5)
C12	0.5164 (2)	0.2695 (3)	0.69118 (6)	0.0365 (5)
C20	0.4639 (2)	0.1076 (3)	0.74128 (6)	0.0352 (5)
C2	0.5645 (2)	0.4436 (2)	0.63805 (6)	0.0322 (5)
H2	0.641392	0.379430	0.630123	0.039*
C11	0.5318 (2)	0.4187 (2)	0.67846 (6)	0.0361 (5)
C4	0.4804 (2)	0.5150 (2)	0.57811 (6)	0.0353 (5)
C21	0.4779 (2)	0.2461 (3)	0.72708 (6)	0.0377 (5)
H21	0.460193	0.323627	0.742761	0.045*
C5	0.5053 (2)	0.6502 (2)	0.60124 (6)	0.0367 (5)
C3	0.4366 (2)	0.4255 (2)	0.61188 (6)	0.0332 (5)
H3	0.413105	0.326134	0.605939	0.040*
C7	0.3144 (2)	0.5104 (3)	0.62806 (6)	0.0409 (5)
H7A	0.299828	0.488296	0.654394	0.049*
H7B	0.226558	0.492847	0.614409	0.049*
C15	0.4932 (2)	−0.0064 (3)	0.71753 (6)	0.0394 (5)
C13	0.5416 (2)	0.1533 (3)	0.66742 (6)	0.0387 (5)
H13	0.565984	0.168661	0.642397	0.046*
C14	0.5307 (2)	0.0201 (3)	0.68070 (7)	0.0408 (5)
H14	0.548878	−0.056467	0.664725	0.049*
C8	0.3638 (3)	0.5307 (3)	0.54932 (7)	0.0499 (6)
H8A	0.282051	0.574768	0.560714	0.075*
H8B	0.337812	0.438197	0.539925	0.075*
H8C	0.397117	0.589021	0.528961	0.075*
C9	0.6120 (3)	0.4631 (3)	0.55838 (6)	0.0426 (6)
H9A	0.640885	0.532133	0.539957	0.064*
H9B	0.591951	0.373884	0.546203	0.064*
H9C	0.687276	0.450052	0.576340	0.064*
C19	0.4206 (3)	0.0829 (3)	0.77769 (7)	0.0438 (6)
H19	0.400420	0.159300	0.793543	0.053*
C16	0.4805 (3)	−0.1453 (3)	0.73169 (8)	0.0496 (6)
H16	0.501686	−0.223071	0.716425	0.060*
C6	0.3646 (3)	0.6628 (3)	0.62289 (7)	0.0442 (6)
H6A	0.379542	0.708616	0.647000	0.053*
H6B	0.295274	0.717616	0.608703	0.053*
C10	0.5525 (3)	0.7813 (3)	0.58164 (7)	0.0523 (7)
H10A	0.565896	0.856496	0.599628	0.078*
H10B	0.481338	0.809412	0.563703	0.078*
H10C	0.640935	0.763122	0.568879	0.078*
C17	0.4383 (3)	−0.1660 (3)	0.76687 (8)	0.0537 (7)
H17	0.429241	−0.258625	0.776009	0.064*
C18	0.4076 (3)	−0.0513 (3)	0.79021 (7)	0.0513 (7)
H18	0.377741	−0.067775	0.814759	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0456 (10)	0.0561 (11)	0.0375 (8)	−0.0160 (8)	−0.0059 (7)	0.0023 (8)
O2	0.0678 (12)	0.0467 (10)	0.0343 (8)	0.0024 (8)	0.0081 (8)	0.0006 (7)
C1	0.0344 (11)	0.0380 (12)	0.0273 (9)	−0.0036 (9)	0.0034 (8)	0.0012 (8)
C12	0.0288 (11)	0.0459 (13)	0.0350 (10)	0.0010 (9)	−0.0009 (9)	0.0071 (9)
C20	0.0255 (10)	0.0455 (13)	0.0345 (10)	−0.0012 (9)	−0.0056 (8)	0.0008 (9)
C2	0.0295 (10)	0.0364 (11)	0.0308 (10)	0.0007 (9)	0.0018 (8)	0.0020 (8)
C11	0.0370 (12)	0.0401 (12)	0.0311 (10)	0.0025 (9)	0.0002 (9)	0.0040 (9)
C4	0.0310 (11)	0.0442 (13)	0.0306 (10)	−0.0031 (9)	−0.0019 (8)	0.0020 (9)
C21	0.0352 (11)	0.0427 (13)	0.0353 (10)	0.0021 (10)	−0.0015 (9)	0.0014 (10)
C5	0.0369 (12)	0.0385 (12)	0.0347 (10)	0.0005 (10)	−0.0007 (9)	0.0052 (9)
C3	0.0290 (11)	0.0370 (11)	0.0337 (10)	−0.0032 (9)	0.0015 (8)	−0.0005 (9)
C7	0.0301 (11)	0.0519 (15)	0.0406 (11)	0.0001 (10)	0.0035 (9)	0.0008 (10)
C15	0.0283 (11)	0.0460 (13)	0.0439 (11)	0.0014 (9)	−0.0072 (9)	0.0020 (10)
C13	0.0353 (12)	0.0439 (13)	0.0370 (11)	0.0023 (10)	0.0012 (9)	0.0007 (10)
C14	0.0351 (12)	0.0441 (13)	0.0432 (11)	0.0052 (10)	−0.0010 (10)	−0.0066 (10)
C8	0.0410 (14)	0.0705 (18)	0.0381 (12)	−0.0032 (13)	−0.0088 (10)	0.0036 (12)
C9	0.0380 (12)	0.0572 (15)	0.0324 (10)	−0.0050 (11)	0.0045 (9)	−0.0035 (10)
C19	0.0396 (13)	0.0527 (15)	0.0390 (11)	−0.0023 (11)	−0.0045 (10)	0.0055 (11)
C16	0.0442 (14)	0.0422 (14)	0.0625 (16)	−0.0025 (11)	−0.0117 (12)	0.0047 (12)
C6	0.0416 (13)	0.0442 (13)	0.0467 (13)	0.0101 (11)	0.0013 (11)	0.0008 (11)
C10	0.0639 (18)	0.0459 (15)	0.0471 (13)	−0.0080 (13)	−0.0071 (12)	0.0129 (11)
C17	0.0502 (16)	0.0447 (14)	0.0662 (16)	−0.0085 (12)	−0.0135 (13)	0.0198 (13)
C18	0.0438 (14)	0.0618 (17)	0.0482 (13)	−0.0051 (12)	−0.0043 (11)	0.0181 (12)

Geometric parameters (Å, º)

O1—C1	1.207 (3)	C7—C6	1.545 (4)
O2—C11	1.213 (3)	C15—C14	1.409 (3)
C1—C2	1.535 (3)	C15—C16	1.430 (4)
C1—C5	1.516 (3)	C13—H13	0.9500
C12—C11	1.507 (3)	C13—C14	1.367 (4)
C12—C21	1.374 (3)	C14—H14	0.9500
C12—C13	1.428 (3)	C8—H8A	0.9800
C20—C21	1.428 (3)	C8—H8B	0.9800
C20—C15	1.418 (3)	C8—H8C	0.9800
C20—C19	1.406 (3)	C9—H9A	0.9800
C2—H2	1.0000	C9—H9B	0.9800
C2—C11	1.521 (3)	C9—H9C	0.9800
C2—C3	1.559 (3)	C19—H19	0.9500
C4—C5	1.560 (3)	C19—C18	1.367 (4)
C4—C3	1.554 (3)	C16—H16	0.9500
C4—C8	1.537 (3)	C16—C17	1.355 (4)
C4—C9	1.531 (3)	C6—H6A	0.9900
C21—H21	0.9500	C6—H6B	0.9900
C5—C6	1.564 (3)	C10—H10A	0.9800

C5—C10	1.511 (3)	C10—H10B	0.9800
C3—H3	1.0000	C10—H10C	0.9800
C3—C7	1.540 (3)	C17—H17	0.9500
C7—H7A	0.9900	C17—C18	1.418 (4)
C7—H7B	0.9900	C18—H18	0.9500

O1—C1—C2	125.9 (2)	C20—C15—C16	118.6 (2)
O1—C1—C5	127.1 (2)	C14—C15—C20	119.4 (2)
C5—C1—C2	106.96 (18)	C14—C15—C16	122.0 (2)
C21—C12—C11	118.1 (2)	C12—C13—H13	120.0
C21—C12—C13	119.5 (2)	C14—C13—C12	120.0 (2)
C13—C12—C11	122.31 (19)	C14—C13—H13	120.0
C15—C20—C21	118.3 (2)	C15—C14—H14	119.3
C19—C20—C21	121.5 (2)	C13—C14—C15	121.5 (2)
C19—C20—C15	120.1 (2)	C13—C14—H14	119.3
C1—C2—H2	109.5	C4—C8—H8A	109.5
C1—C2—C3	101.15 (16)	C4—C8—H8B	109.5
C11—C2—C1	112.83 (18)	C4—C8—H8C	109.5
C11—C2—H2	109.5	H8A—C8—H8B	109.5
C11—C2—C3	114.20 (17)	H8A—C8—H8C	109.5
C3—C2—H2	109.5	H8B—C8—H8C	109.5
O2—C11—C12	121.90 (19)	C4—C9—H9A	109.5
O2—C11—C2	120.4 (2)	C4—C9—H9B	109.5
C12—C11—C2	117.72 (19)	C4—C9—H9C	109.5
C3—C4—C5	94.14 (16)	H9A—C9—H9B	109.5
C8—C4—C5	113.4 (2)	H9A—C9—H9C	109.5
C8—C4—C3	113.29 (19)	H9B—C9—H9C	109.5
C9—C4—C5	113.31 (19)	C20—C19—H19	120.1
C9—C4—C3	114.39 (19)	C18—C19—C20	119.8 (3)
C9—C4—C8	108.02 (19)	C18—C19—H19	120.1
C12—C21—C20	121.3 (2)	C15—C16—H16	120.0
C12—C21—H21	119.4	C17—C16—C15	120.1 (3)
C20—C21—H21	119.4	C17—C16—H16	120.0
C1—C5—C4	100.46 (18)	C5—C6—H6A	110.8
C1—C5—C6	103.31 (18)	C5—C6—H6B	110.8
C4—C5—C6	101.74 (18)	C7—C6—C5	104.83 (19)
C10—C5—C1	114.8 (2)	C7—C6—H6A	110.8
C10—C5—C4	118.64 (19)	C7—C6—H6B	110.8
C10—C5—C6	115.5 (2)	H6A—C6—H6B	108.9
C2—C3—H3	114.4	C5—C10—H10A	109.5
C4—C3—C2	102.03 (16)	C5—C10—H10B	109.5
C4—C3—H3	114.4	C5—C10—H10C	109.5
C7—C3—C2	107.70 (17)	H10A—C10—H10B	109.5
C7—C3—C4	102.45 (18)	H10A—C10—H10C	109.5
C7—C3—H3	114.4	H10B—C10—H10C	109.5
C3—C7—H7A	111.3	C16—C17—H17	119.6
C3—C7—H7B	111.3	C16—C17—C18	120.8 (3)
C3—C7—C6	102.44 (18)	C18—C17—H17	119.6

H7A—C7—H7B	109.2	C19—C18—C17	120.6 (2)
C6—C7—H7A	111.3	C19—C18—H18	119.7
C6—C7—H7B	111.3	C17—C18—H18	119.7
O1—C1—C2—C11	58.5 (3)	C5—C4—C3—C2	−55.30 (19)
O1—C1—C2—C3	−179.1 (2)	C5—C4—C3—C7	56.14 (19)
O1—C1—C5—C4	144.2 (2)	C3—C2—C11—O2	−101.7 (3)
O1—C1—C5—C6	−110.9 (3)	C3—C2—C11—C12	76.7 (3)
O1—C1—C5—C10	15.7 (3)	C3—C4—C5—C1	54.17 (19)
C1—C2—C11—O2	13.1 (3)	C3—C4—C5—C6	−51.94 (19)
C1—C2—C11—C12	−168.51 (19)	C3—C4—C5—C10	−179.9 (2)
C1—C2—C3—C4	35.2 (2)	C3—C7—C6—C5	4.6 (2)
C1—C2—C3—C7	−72.2 (2)	C15—C20—C21—C12	1.1 (3)
C1—C5—C6—C7	−73.3 (2)	C15—C20—C19—C18	0.4 (3)
C12—C13—C14—C15	0.8 (4)	C15—C16—C17—C18	−0.6 (4)
C20—C15—C14—C13	1.0 (3)	C13—C12—C11—O2	−176.8 (2)
C20—C15—C16—C17	1.4 (4)	C13—C12—C11—C2	4.8 (3)
C20—C19—C18—C17	0.4 (4)	C13—C12—C21—C20	0.6 (3)
C2—C1—C5—C4	−34.7 (2)	C14—C15—C16—C17	−177.2 (2)
C2—C1—C5—C6	70.1 (2)	C8—C4—C5—C1	171.77 (19)
C2—C1—C5—C10	−163.2 (2)	C8—C4—C5—C6	65.7 (2)
C2—C3—C7—C6	68.6 (2)	C8—C4—C5—C10	−62.3 (3)
C11—C12—C21—C20	−178.8 (2)	C8—C4—C3—C2	−172.96 (19)
C11—C12—C13—C14	177.8 (2)	C8—C4—C3—C7	−61.5 (2)
C11—C2—C3—C4	156.71 (18)	C9—C4—C5—C1	−64.6 (2)
C11—C2—C3—C7	49.3 (2)	C9—C4—C5—C6	−170.76 (18)
C4—C5—C6—C7	30.5 (2)	C9—C4—C5—C10	61.3 (3)
C4—C3—C7—C6	−38.6 (2)	C9—C4—C3—C2	62.6 (2)
C21—C12—C11—O2	2.6 (3)	C9—C4—C3—C7	174.07 (19)
C21—C12—C11—C2	−175.8 (2)	C19—C20—C21—C12	−178.1 (2)
C21—C12—C13—C14	−1.6 (3)	C19—C20—C15—C14	177.3 (2)
C21—C20—C15—C14	−1.9 (3)	C19—C20—C15—C16	−1.3 (3)
C21—C20—C15—C16	179.5 (2)	C16—C15—C14—C13	179.6 (2)
C21—C20—C19—C18	179.6 (2)	C16—C17—C18—C19	−0.3 (4)
C5—C1—C2—C11	−122.51 (19)	C10—C5—C6—C7	160.4 (2)
C5—C1—C2—C3	−0.1 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O1^{i}	0.95	2.57	3.296 (3)	134
C16—H16···O2^{ii}	0.95	2.57	3.458 (3)	156

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+5/4; (ii) *x*, *y*−1, *z*.