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4-Methyl-2,6-bis(2-naphthylmethylene)-cyclohexan-1-one

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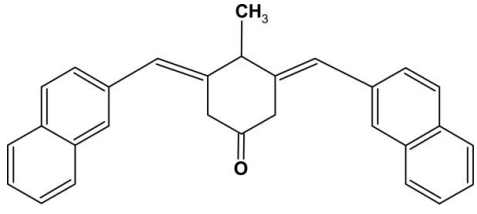
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.008 Å; R factor = 0.040; wR factor = 0.115; data-to-parameter ratio = 10.5.

The molecular skeleton of the title molecule, $C_{29}H_{24}O$, has a 'bird-like' general conformation. The naphthyl units ('wings') make a dihedral angle of 46.1 (1)°. The central cyclohexanone ring adopts an envelope conformation.

Related literature

For details of structure–activity correlations in related 3,5-bis(arylidene)-4-piperidones, see: Dimmock *et al.* (2001). For details of highly active curcumin derivatives used as anti-cancer agents, see: Dimmock *et al.* (2005). For details of conformational analysis in organic molecules, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{29}H_{24}O$
M_r = 388.48
Monoclinic, $P2_1/n$
a = 14.5282 (19) Å
b = 10.3604 (14) Å
c = 14.708 (2) Å
β = 103.312 (3)°
V = 2154.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 290 (2) K
0.25 × 0.21 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.936, T_{max} = 0.986
16027 measured reflections
4081 independent reflections
2777 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.115
S = 1.02
4081 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2324).

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supplementary materials

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4-Methyl-2,6-bis(2-naphthylmethylene)cyclohexan-1-one

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Comment

Substituted 2,6-bis(benzylidenecyclohexanone) derivatives have been the subject of recent crystallographic investigations and have found useful applications as potent anti-cancer agents (Dimmock *et al.*, 2001, 2005).

In the title compound (Fig. 1), the six-membered cyclohexanone ring exists in an envelope conformation, the Cremer and Pople puckering parameters are Q(T) = 0.414 (6) Å, φ(2) = 166.2 (12)°, θ (2) = 40.8 (8)° (Cremer and Pople, 1975). Atom C4 deviates at −0.541 (6) Å from the least squares plane C1/C2/C3/C5/C6. Two bicycles make a dihedral angle of 46.1 (1)°.

The crystal structure is stabilized by van-der Waals interactions.

Experimental

An aqueous solution of sodium hydroxide (10% *w*/*v*, 30 ml) was added to a solution of 1-naphthaldehyde (2.7 ml, 0.02 mol) and /g-methylcyclohexanone (1.3 mL, 0.01 mol) in ethanol (50 ml). The reaction mixture was stirred at 10–20 °C for 2 h and left overnight in an ice chest to get a yellow coloured solid. The product was filtered, washed with ice-cold water (100 ml) followed by ice-cold ethanol (20 ml), dried and recrystallized from DMF. Yield: 78%, m.p.: 172–173%C.

Refinement

All H atoms were geometrically positioned (C—H 0.93–0.98 Å) and refined as riding, with U_{iso}(H) = 1.2–1.5U_{eq}(C).

Figures

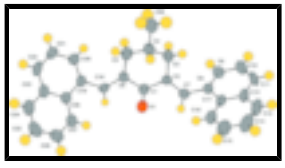


Fig. 1. Molecular structure of the title compound with the atomic numbering and 50% probability displacement ellipsoids.

4-Methyl-2,6-bis(2-naphthylmethylene)cyclohexan-1-one

Crystal data

$C_{29}H_{24}O$	F_{000} = 824
M_r = 388.48	D_x = 1.198 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 4081 reflections
a = 14.5282 (19) Å	θ = 1.8–20.8º

b = 10.3604 (14) Å	μ = 0.07 mm^{-1}
c = 14.708 (2) Å	T = 290 (2) K
β = 103.312 (3)º	Blocks, yellow
V = 2154.3 (5) Å^3	0.25 × 0.21 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2777 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.060
T = 290(2) K	θ_{max} = 25.7º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1997)	h = −17→17
T_{min} = 0.936, T_{max} = 0.986	k = −12→12
16027 measured reflections	l = −17→17
4081 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained
$wR(F^2)$ = 0.115	$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.2955P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
4081 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
272 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}

O1	0.3468 (3)	0.0948 (3)	0.0205 (3)	0.0639 (11)
C1	0.4037 (3)	0.0337 (5)	0.0777 (3)	0.0412 (12)
C2	0.4101 (3)	−0.1100 (5)	0.0694 (3)	0.0394 (11)
C3	0.4969 (4)	−0.1763 (5)	0.1248 (4)	0.0552 (14)
C4	0.5323 (4)	−0.1192 (5)	0.2193 (4)	0.0662 (17)
C5	0.5494 (4)	0.0216 (5)	0.2167 (4)	0.0653 (17)
C6	0.4692 (3)	0.0994 (5)	0.1582 (3)	0.0421 (12)
C7	0.3361 (3)	−0.1704 (5)	0.0189 (3)	0.0461 (13)
C8	0.3266 (4)	−0.3101 (5)	−0.0015 (3)	0.0450 (13)
C9	0.3891 (4)	−0.3702 (6)	−0.0443 (4)	0.0616 (15)
C10	0.3796 (5)	−0.4999 (6)	−0.0696 (4)	0.0718 (18)
C11	0.3085 (5)	−0.5711 (5)	−0.0505 (4)	0.0683 (18)
C12	0.2428 (4)	−0.5160 (5)	−0.0046 (3)	0.0538 (15)
C13	0.1679 (5)	−0.5875 (6)	0.0172 (4)	0.0755 (19)
C14	0.1065 (6)	−0.5327 (7)	0.0625 (5)	0.088 (2)
C15	0.1150 (5)	−0.4025 (7)	0.0865 (5)	0.081 (2)
C16	0.1852 (4)	−0.3292 (6)	0.0664 (4)	0.0585 (15)
C17	0.2509 (4)	−0.3836 (5)	0.0200 (3)	0.0462 (13)
C18	0.4495 (3)	0.2222 (5)	0.1732 (3)	0.0408 (12)
C19	0.4976 (4)	0.3126 (5)	0.2461 (3)	0.0440 (12)
C20	0.5936 (4)	0.3138 (5)	0.2784 (4)	0.0541 (14)
C21	0.6382 (4)	0.4012 (6)	0.3464 (4)	0.0644 (16)
C22	0.5872 (5)	0.4890 (6)	0.3820 (4)	0.0700 (18)
C23	0.4884 (4)	0.4944 (5)	0.3510 (4)	0.0568 (15)
C24	0.4337 (5)	0.5854 (7)	0.3875 (5)	0.084 (2)
C25	0.3390 (6)	0.5889 (7)	0.3578 (5)	0.087 (2)
C26	0.2932 (5)	0.5019 (6)	0.2914 (5)	0.0755 (19)
C27	0.3427 (4)	0.4130 (5)	0.2546 (4)	0.0562 (14)
C28	0.4417 (4)	0.4056 (5)	0.2825 (3)	0.0465 (13)
C29	0.6199 (5)	−0.1892 (6)	0.2752 (5)	0.095 (2)
H3A	0.4827	−0.2667	0.1315	0.066*
H3B	0.5464	−0.1713	0.0906	0.066*
H4	0.4823	−0.1313	0.2532	0.079*
H5A	0.6055	0.0357	0.1928	0.078*
H5B	0.5626	0.0544	0.2801	0.078*
H7	0.2839	−0.1195	−0.0069	0.055*
H9	0.4392	−0.3232	−0.0569	0.074*
H10	0.4224	−0.5376	−0.0998	0.086*
H11	0.3028	−0.6576	−0.0678	0.082*
H13	0.1605	−0.6739	0.0000	0.091*
H14	0.0586	−0.5821	0.0775	0.106*
H15	0.0720	−0.3653	0.1167	0.098*
H16	0.1901	−0.2426	0.0833	0.070*
H18	0.3973	0.2560	0.1311	0.049*
H20	0.6301	0.2549	0.2544	0.065*
H21	0.7036	0.3991	0.3675	0.077*
H22	0.6179	0.5465	0.4275	0.084*
H24	0.4638	0.6437	0.4328	0.101*
H27	0.3103	0.3556	0.2099	0.067*

H25	0.3043	0.6500	0.3819	0.105*
H26	0.2277	0.5045	0.2717	0.091*
H29A	0.6097	−0.2808	0.2703	0.143*
H29B	0.6313	−0.1638	0.3396	0.143*
H29C	0.6737	−0.1671	0.2508	0.143*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.071 (3)	0.040 (2)	0.064 (2)	0.0018 (19)	−0.019 (2)	0.0077 (19)
C1	0.042 (3)	0.041 (3)	0.041 (3)	−0.004 (2)	0.011 (2)	0.005 (2)
C2	0.038 (3)	0.042 (3)	0.037 (3)	0.002 (2)	0.004 (2)	−0.002 (2)
C3	0.059 (4)	0.046 (3)	0.058 (3)	−0.001 (3)	0.009 (3)	−0.007 (3)
C4	0.077 (4)	0.046 (4)	0.065 (4)	0.007 (3)	−0.005 (3)	0.001 (3)
C5	0.066 (4)	0.055 (4)	0.062 (4)	0.000 (3)	−0.010 (3)	−0.002 (3)
C6	0.044 (3)	0.035 (3)	0.048 (3)	−0.002 (2)	0.011 (2)	0.000 (2)
C7	0.042 (3)	0.044 (3)	0.049 (3)	0.004 (2)	0.005 (2)	0.001 (2)
C8	0.049 (3)	0.037 (3)	0.041 (3)	0.002 (2)	−0.006 (2)	−0.001 (2)
C9	0.058 (4)	0.054 (4)	0.071 (4)	0.003 (3)	0.011 (3)	−0.007 (3)
C10	0.078 (5)	0.058 (4)	0.081 (4)	0.009 (4)	0.021 (4)	−0.019 (3)
C11	0.096 (5)	0.031 (3)	0.069 (4)	0.016 (3)	0.000 (4)	−0.009 (3)
C12	0.073 (4)	0.037 (3)	0.042 (3)	−0.008 (3)	−0.006 (3)	0.000 (2)
C13	0.103 (5)	0.053 (4)	0.062 (4)	−0.027 (4)	0.001 (4)	0.002 (3)
C14	0.101 (6)	0.085 (6)	0.080 (5)	−0.047 (5)	0.024 (4)	−0.001 (4)
C15	0.083 (5)	0.088 (5)	0.080 (5)	−0.023 (4)	0.032 (4)	−0.011 (4)
C16	0.068 (4)	0.056 (4)	0.050 (3)	−0.010 (3)	0.009 (3)	−0.009 (3)
C17	0.056 (3)	0.045 (3)	0.030 (2)	−0.005 (3)	−0.008 (2)	−0.003 (2)
C18	0.032 (3)	0.043 (3)	0.046 (3)	−0.004 (2)	0.005 (2)	0.002 (2)
C19	0.051 (3)	0.032 (3)	0.046 (3)	−0.006 (2)	0.006 (2)	0.006 (2)
C20	0.047 (3)	0.046 (3)	0.065 (4)	−0.002 (3)	0.004 (3)	0.002 (3)
C21	0.052 (4)	0.055 (4)	0.073 (4)	−0.009 (3)	−0.011 (3)	−0.001 (3)
C22	0.081 (5)	0.053 (4)	0.063 (4)	−0.019 (3)	−0.011 (3)	−0.015 (3)
C23	0.070 (4)	0.043 (3)	0.054 (3)	−0.005 (3)	0.006 (3)	−0.006 (3)
C24	0.096 (6)	0.071 (5)	0.077 (5)	−0.003 (4)	0.000 (4)	−0.029 (4)
C25	0.104 (6)	0.070 (5)	0.087 (5)	0.021 (4)	0.021 (4)	−0.018 (4)
C26	0.071 (4)	0.073 (4)	0.081 (4)	0.014 (4)	0.012 (4)	−0.008 (4)
C27	0.064 (4)	0.047 (3)	0.055 (3)	0.002 (3)	0.008 (3)	−0.005 (3)
C28	0.054 (3)	0.036 (3)	0.047 (3)	−0.004 (2)	0.005 (2)	0.008 (2)
C29	0.109 (6)	0.061 (4)	0.085 (5)	0.022 (4)	−0.039 (4)	0.001 (4)

Geometric parameters (Å, °)

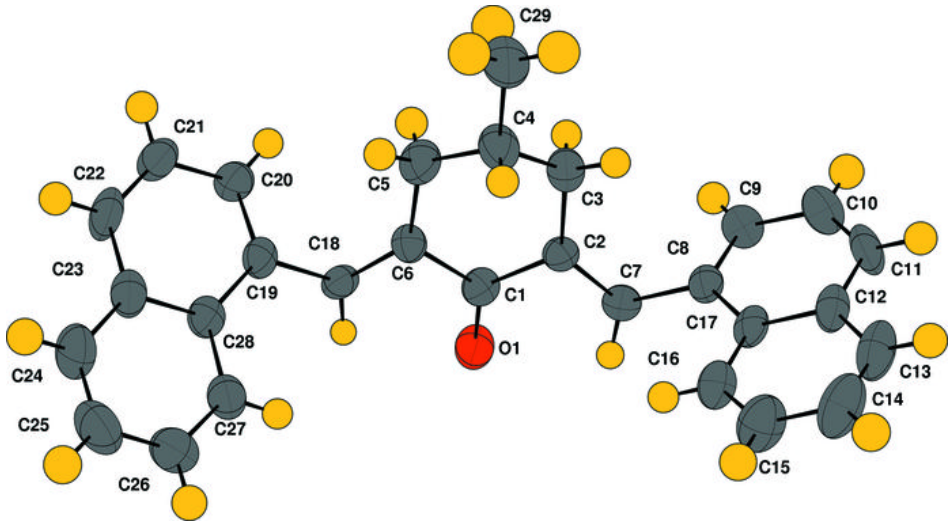
O1—C1	1.213 (5)	C5—H5B	0.9700
C28—C27	1.404 (7)	C3—C4	1.488 (7)
C28—C23	1.416 (7)	C3—H3A	0.9700
C28—C19	1.441 (7)	C3—H3B	0.9700
C17—C16	1.412 (7)	C4—C29	1.530 (7)
C17—C12	1.417 (7)	C4—H4	0.9800
C17—C8	1.432 (7)	C20—C21	1.394 (7)

C1—C2	1.498 (7)	C20—H20	0.9300
C1—C6	1.501 (6)	C9—C10	1.392 (8)
C7—C2	1.316 (6)	C9—H9	0.9300
C7—C8	1.478 (7)	C23—C22	1.403 (8)
C7—H7	0.9300	C23—C24	1.417 (8)
C2—C3	1.502 (6)	C13—C14	1.355 (9)
C8—C9	1.368 (7)	C13—H13	0.9300
C12—C11	1.411 (8)	C21—C22	1.353 (8)
C12—C13	1.413 (8)	C21—H21	0.9300
C6—C18	1.334 (6)	C22—H22	0.9300
C6—C5	1.512 (7)	C24—C25	1.345 (9)
C19—C20	1.365 (7)	C24—H24	0.9300
C19—C18	1.474 (6)	C14—C15	1.393 (9)
C18—H18	0.9300	C14—H14	0.9300
C16—C15	1.358 (8)	C25—C26	1.381 (9)
C16—H16	0.9300	C25—H25	0.9300
C11—C10	1.351 (8)	C26—H26	0.9300
C11—H11	0.9300	C29—H29A	0.9600
C27—C26	1.355 (8)	C29—H29B	0.9600
C27—H27	0.9300	C29—H29C	0.9600
C5—C4	1.482 (8)	C15—H15	0.9300
C5—H5A	0.9700	C10—H10	0.9300
C27—C28—C23	117.6 (5)	H3A—C3—H3B	107.8
C27—C28—C19	123.8 (5)	C5—C4—C3	113.0 (5)
C23—C28—C19	118.6 (5)	C5—C4—C29	110.9 (5)
C16—C17—C12	118.9 (5)	C3—C4—C29	112.3 (5)
C16—C17—C8	122.3 (5)	C5—C4—H4	106.7
C12—C17—C8	118.8 (5)	C3—C4—H4	106.7
O1—C1—C2	120.5 (4)	C29—C4—H4	106.7
O1—C1—C6	121.1 (4)	C19—C20—C21	121.6 (5)
C2—C1—C6	118.4 (4)	C19—C20—H20	119.2
C2—C7—C8	127.3 (5)	C21—C20—H20	119.2
C2—C7—H7	116.3	C8—C9—C10	121.8 (6)
C8—C7—H7	116.3	C8—C9—H9	119.1
C7—C2—C1	117.5 (4)	C10—C9—H9	119.1
C7—C2—C3	124.3 (5)	C22—C23—C28	119.5 (5)
C1—C2—C3	118.1 (4)	C22—C23—C24	121.6 (6)
C9—C8—C17	119.0 (5)	C28—C23—C24	118.9 (6)
C9—C8—C7	119.9 (5)	C14—C13—C12	121.4 (6)
C17—C8—C7	121.0 (5)	C14—C13—H13	119.3
C11—C12—C13	122.6 (6)	C12—C13—H13	119.3
C11—C12—C17	119.2 (5)	C22—C21—C20	120.6 (5)
C13—C12—C17	118.2 (6)	C22—C21—H21	119.7
C18—C6—C1	116.2 (4)	C20—C21—H21	119.7
C18—C6—C5	125.5 (5)	C21—C22—C23	120.8 (5)
C1—C6—C5	118.2 (4)	C21—C22—H22	119.6
C20—C19—C28	118.9 (5)	C23—C22—H22	119.6
C20—C19—C18	122.3 (5)	C25—C24—C23	121.0 (6)
C28—C19—C18	118.8 (4)	C25—C24—H24	119.5

C6—C18—C19	130.0 (5)	C23—C24—H24	119.5
C6—C18—H18	115.0	C13—C14—C15	120.0 (6)
C19—C18—H18	115.0	C13—C14—H14	120.0
C15—C16—C17	120.5 (6)	C15—C14—H14	120.0
C15—C16—H16	119.8	C24—C25—C26	120.2 (6)
C17—C16—H16	119.8	C24—C25—H25	119.9
C10—C11—C12	120.9 (5)	C26—C25—H25	119.9
C10—C11—H11	119.6	C27—C26—C25	120.8 (6)
C12—C11—H11	119.6	C27—C26—H26	119.6
C26—C27—C28	121.5 (5)	C25—C26—H26	119.6
C26—C27—H27	119.3	C4—C29—H29A	109.5
C28—C27—H27	119.3	C4—C29—H29B	109.5
C4—C5—C6	115.3 (5)	H29A—C29—H29B	109.5
C4—C5—H5A	108.5	C4—C29—H29C	109.5
C6—C5—H5A	108.5	H29A—C29—H29C	109.5
C4—C5—H5B	108.5	H29B—C29—H29C	109.5
C6—C5—H5B	108.5	C16—C15—C14	120.9 (7)
H5A—C5—H5B	107.5	C16—C15—H15	119.5
C4—C3—C2	113.1 (4)	C14—C15—H15	119.5
C4—C3—H3A	109.0	C11—C10—C9	120.3 (6)
C2—C3—H3A	109.0	C11—C10—H10	119.8
C4—C3—H3B	109.0	C9—C10—H10	119.8
C2—C3—H3B	109.0		
C8—C7—C2—C1	178.2 (5)	C19—C28—C27—C26	179.6 (5)
C8—C7—C2—C3	−6.7 (8)	C18—C6—C5—C4	150.9 (5)
O1—C1—C2—C7	−20.8 (7)	C1—C6—C5—C4	−27.3 (7)
C6—C1—C2—C7	159.1 (4)	C7—C2—C3—C4	−137.2 (5)
O1—C1—C2—C3	163.7 (5)	C1—C2—C3—C4	37.9 (7)
C6—C1—C2—C3	−16.4 (6)	C6—C5—C4—C3	49.4 (8)
C16—C17—C8—C9	178.2 (5)	C6—C5—C4—C29	176.5 (5)
C12—C17—C8—C9	−0.5 (7)	C2—C3—C4—C5	−54.4 (7)
C16—C17—C8—C7	−3.9 (7)	C2—C3—C4—C29	179.1 (5)
C12—C17—C8—C7	177.4 (4)	C28—C19—C20—C21	1.1 (8)
C2—C7—C8—C9	−57.8 (7)	C18—C19—C20—C21	179.0 (5)
C2—C7—C8—C17	124.4 (6)	C17—C8—C9—C10	1.6 (8)
C16—C17—C12—C11	−179.7 (5)	C7—C8—C9—C10	−176.3 (5)
C8—C17—C12—C11	−0.9 (7)	C27—C28—C23—C22	178.9 (5)
C16—C17—C12—C13	1.1 (7)	C19—C28—C23—C22	−0.4 (8)
C8—C17—C12—C13	179.9 (5)	C27—C28—C23—C24	−0.1 (8)
O1—C1—C6—C18	12.2 (7)	C19—C28—C23—C24	−179.5 (5)
C2—C1—C6—C18	−167.7 (4)	C11—C12—C13—C14	179.1 (6)
O1—C1—C6—C5	−169.4 (5)	C17—C12—C13—C14	−1.7 (9)
C2—C1—C6—C5	10.8 (7)	C19—C20—C21—C22	−0.7 (9)
C27—C28—C19—C20	−179.8 (5)	C20—C21—C22—C23	−0.3 (9)
C23—C28—C19—C20	−0.5 (7)	C28—C23—C22—C21	0.8 (9)
C27—C28—C19—C18	2.2 (7)	C24—C23—C22—C21	179.9 (6)
C23—C28—C19—C18	−178.5 (4)	C22—C23—C24—C25	−179.5 (7)
C1—C6—C18—C19	178.7 (4)	C28—C23—C24—C25	−0.4 (10)
C5—C6—C18—C19	0.5 (8)	C12—C13—C14—C15	1.7 (10)

C20—C19—C18—C6	36.9 (8)	C23—C24—C25—C26	0.8 (11)
C28—C19—C18—C6	−145.1 (5)	C28—C27—C26—C25	0.1 (9)
C12—C17—C16—C15	−0.5 (8)	C24—C25—C26—C27	−0.7 (11)
C8—C17—C16—C15	−179.2 (5)	C17—C16—C15—C14	0.4 (10)
C13—C12—C11—C10	−179.6 (6)	C13—C14—C15—C16	−1.0 (11)
C17—C12—C11—C10	1.2 (8)	C12—C11—C10—C9	−0.1 (9)
C23—C28—C27—C26	0.3 (8)	C8—C9—C10—C11	−1.3 (9)

Fig. 1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