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2,3-Dibromo-3-(5-bromo-6-methoxy-2-naphthyl)-1-(2,4-dichlorophenyl)propan-1-one

H. S. Yathirajan,[a] Anil M. Mayekar,[a] B. Narayana,[b] B. K. Sarojini[c] and Michael Bolte[d]*

[a]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, [b]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, India, [c]Department of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and [d]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany
Correspondence e-mail: bolte@chemie.uni-frankfurt.de

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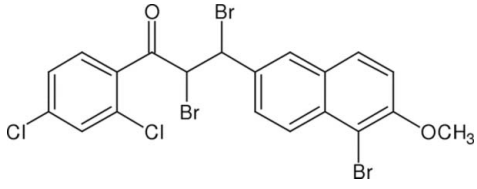
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.095; data-to-parameter ratio = 22.6.

The title compound, $C_{20}H_{13}Br_3Cl_2O_2$, arose unexpectedly as the product of a bromination reaction. The bromo substituents at the central C—C single bond are *trans* to each other [Br—C—C—Br = 178.53 (13)°] and the dihedral angle between the mean planes of the aromatic ring systems is 38.28 (10)°.

Related literature

For some recent crystal structures of related chalcones, see: Butcher, Yathirajan, Anilkumar *et al.* (2006); Butcher, Yathirajan, Sarojini *et al.* (2006); Harrison *et al.* (2005); Yathirajan *et al.* (2007); Allen (2002); Bruno *et al.* (2004).



Experimental

Crystal data

$C_{20}H_{13}Br_3Cl_2O_2$
M_r = 595.93
Monoclinic, $P2_1/n$
a = 9.3506 (4) Å
b = 9.8861 (5) Å
c = 21.7179 (9) Å
β = 98.298 (3)°
V = 1986.61 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.38 mm^{-1}
T = 173 (2) K
0.23 × 0.22 × 0.20 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.236, T_{max} = 0.263 (expected range = 0.251–0.279)
30941 measured reflections
5563 independent reflections
4864 reflections with $I > 2\sigma(I)$
R_{int} = 0.070

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.095
S = 1.04
5563 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

Table 1
Selected torsion angles (°).

Br2—C2—C3—Br3	178.53 (13)	O1—C1—C11—C12	−41.1 (4)

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

ANM thanks the University of Mysore for permission to carry out the research work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2359).

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supplementary materials

Acta Cryst. (2007). E**63**, o2345 [**doi:10.1107/S1600536807015759**]

2,3-Dibromo-3-(5-bromo-6-methoxy-2-naphthyl)-1-(2,4-dichlorophenyl)propan-1-one

H. S. Yathirajan, A. M. Mayekar, B. Narayana, B. K. Sarojini and M. Bolte

Comment

The title compound, (I), was obtained as an unexpected product in a bromination reaction. The expected compound was 2,3-dibromo-3-(6-methoxy-2-naphthyl)-1-(2,4-dichlorophenyl)propan-1-one which reacted further with excess bromine to form 2,3-dibromo-3-(5-bromo-6-methoxy-2-naphthyl)-1-(2,4-dichlorophenyl)propan-1-one.

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Crystallographic Database, Version 5.28, November 2006; updated January 2007; Mogul Version 1.1; Allen, 2002, Bruno *et al.*, 2004). The bromo substituents at the central C—C single bond are trans to each other and the carbonyl group is is twisted by -41.1 (4)° out of the plane of the adjacent dichlorophenyl ring. The two aromatic ring systems are not coplanar [dihedral angle 38.28 (10)°].

For structures of related chalcones see Harrison *et al.* (2005, Butcher *et al.* (2006a,b) and Yathirajan *et al.* (2007).

Experimental

(2E)-1-(2,4-Dichlorophenyl)-3-(6-methoxy-2-naphthyl)prop-2-en-1-one (3.57 g, 0.01 mol) was treated with bromine in acetic acid (30%) until the orange colour of the solution persisted. After stirring for half an hour, the contents were poured on to crushed ice. The resulting solid mass was collected by filtration. The compound was dried and recrystallized from ethanol. Crystals of (I) suitable for structure determination were obtained from acetone by slow evaporation (yield 80%; m.p. 439-441 K). Analysis for $C_{20}H_{13}Br_3Cl_2O_2$: found (calculated): C 40.20 (40.31%); H 2.14 (2.20%).

Refinement

The H atoms were found in a difference map, relocated in idealised locations (C—H = 0.95-1.00 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C_{methyl})$. The methyl

group was allowed to rotate but not to tip to best fit the electron density.

Figures

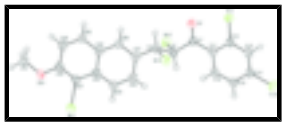


Fig. 1. Perspective view of (I) with the atom numbering; displacement ellipsoids are at the 50% probability level (arbitrary spheres for the H atoms).

2,3-Dibromo-3-(5-bromo-6-methoxy-2-naphthyl)-1-(2,4-dichlorophenyl)propan-1-one

Crystal data

$C_{20}H_{13}Br_3Cl_2O_2$	F_{000} = 1152
M_r = 595.93	D_x = 1.992 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 30108 reflections
a = 9.3506 (4) Å	θ = 2.8–28.8º
b = 9.8861 (5) Å	μ = 6.38 mm^{-1}
c = 21.7179 (9) Å	T = 173 (2) K
β = 98.298 (3)º	Block, light yellow
V = 1986.61 (16) Å^3	0.23 × 0.22 × 0.20 mm
Z = 4	

Data collection

Stoe IPDSII two-circle diffractometer	5563 independent reflections
Radiation source: fine-focus sealed tube	4864 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.070
T = 173(2) K	θ_{max} = 29.7º
ω scans	θ_{min} = 2.8º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	h = −12→11
T_{min} = 0.236, T_{max} = 0.263	k = −13→13
30941 measured reflections	l = −30→30

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 1.8115P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$(\Delta/\sigma)_{max}$ = 0.002
$wR(F^2)$ = 0.095	$\Delta\rho_{max}$ = 0.64 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.75 e Å^{-3}
5563 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
246 parameters	Extinction coefficient: 0.0064 (4)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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. 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	0.8339 (3)	1.0876 (2)	0.72563 (10)	0.0356 (5)
Cl1	1.12598 (8)	0.97308 (8)	0.78146 (3)	0.03755 (17)
Cl2	1.03476 (9)	0.81388 (8)	1.00892 (3)	0.03864 (17)
Br1	−0.05973 (3)	0.64021 (3)	0.547822 (14)	0.03635 (9)
Br2	0.74588 (3)	0.79954 (3)	0.654006 (13)	0.03479 (9)
Br3	0.46605 (4)	1.10035 (4)	0.748535 (15)	0.04018 (10)
C1	0.7893 (3)	0.9882 (3)	0.74980 (12)	0.0291 (5)
C2	0.6601 (3)	0.9090 (3)	0.71527 (12)	0.0293 (5)
H2	0.6169	0.8492	0.7448	0.035*
C3	0.5455 (3)	1.0008 (3)	0.68072 (13)	0.0319 (6)
H3	0.5936	1.0672	0.6556	0.038*
C11	0.8542 (3)	0.9380 (3)	0.81242 (12)	0.0286 (5)
C12	1.0039 (3)	0.9343 (3)	0.83201 (13)	0.0291 (5)
C13	1.0609 (3)	0.8940 (3)	0.89222 (13)	0.0325 (6)
H13	1.1624	0.8890	0.9047	0.039*
C14	0.9656 (3)	0.8615 (3)	0.93321 (13)	0.0321 (6)
C15	0.8175 (3)	0.8649 (3)	0.91599 (13)	0.0328 (6)
H15	0.7541	0.8423	0.9449	0.039*
C16	0.7638 (3)	0.9019 (3)	0.85572 (13)	0.0316 (6)
H16	0.6621	0.9030	0.8433	0.038*
C21	0.4232 (3)	0.9357 (3)	0.63943 (13)	0.0319 (6)
C22	0.3423 (4)	0.8275 (3)	0.66015 (14)	0.0362 (6)
H22	0.3696	0.7916	0.7007	0.043*
C23	0.2261 (3)	0.7744 (3)	0.62292 (14)	0.0343 (6)
H23	0.1731	0.7030	0.6383	0.041*
C24	0.1825 (3)	0.8239 (3)	0.56133 (12)	0.0281 (5)
C25	0.2662 (3)	0.9305 (3)	0.53973 (12)	0.0297 (5)
C26	0.3855 (3)	0.9840 (3)	0.57971 (13)	0.0314 (6)
H26	0.4408	1.0547	0.5652	0.038*
C27	0.0616 (3)	0.7750 (3)	0.52019 (13)	0.0293 (5)
C28	0.0269 (3)	0.8237 (3)	0.46020 (13)	0.0305 (5)
C29	0.1124 (3)	0.9287 (3)	0.43966 (13)	0.0338 (6)
H29	0.0893	0.9636	0.3987	0.041*

C30	0.2277 (3)	0.9800 (3)	0.47850 (13)	0.0321 (6)
H30	0.2833	1.0506	0.4640	0.039*
O31	−0.0872 (2)	0.7671 (3)	0.42291 (10)	0.0377 (5)
C31	−0.1160 (4)	0.8144 (4)	0.35984 (14)	0.0421 (7)
H31A	−0.1427	0.9102	0.3596	0.063*
H31B	−0.1956	0.7620	0.3371	0.063*
H31C	−0.0293	0.8031	0.3398	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0350 (11)	0.0367 (11)	0.0352 (10)	−0.0030 (9)	0.0054 (9)	0.0042 (8)
Cl1	0.0301 (3)	0.0462 (4)	0.0379 (3)	−0.0003 (3)	0.0102 (3)	0.0037 (3)
Cl2	0.0445 (4)	0.0410 (4)	0.0282 (3)	0.0026 (3)	−0.0020 (3)	0.0026 (3)
Br1	0.03615 (17)	0.03848 (17)	0.03545 (15)	−0.00812 (12)	0.00867 (12)	−0.00269 (11)
Br2	0.03989 (17)	0.03451 (16)	0.02969 (14)	0.00460 (12)	0.00409 (11)	−0.00076 (10)
Br3	0.03334 (17)	0.0458 (2)	0.04089 (17)	0.00262 (13)	0.00360 (12)	−0.01018 (13)
C1	0.0293 (14)	0.0315 (13)	0.0266 (11)	0.0002 (11)	0.0044 (10)	−0.0010 (10)
C2	0.0296 (13)	0.0327 (14)	0.0257 (11)	0.0005 (11)	0.0042 (10)	−0.0003 (10)
C3	0.0333 (15)	0.0336 (14)	0.0281 (12)	0.0005 (11)	0.0019 (10)	−0.0005 (10)
C11	0.0277 (13)	0.0301 (13)	0.0276 (11)	−0.0024 (10)	0.0020 (10)	−0.0002 (10)
C12	0.0277 (13)	0.0316 (13)	0.0285 (12)	0.0001 (11)	0.0056 (10)	−0.0017 (10)
C13	0.0291 (14)	0.0368 (15)	0.0308 (13)	0.0004 (11)	0.0013 (11)	−0.0033 (11)
C14	0.0370 (15)	0.0312 (14)	0.0269 (12)	0.0002 (11)	0.0008 (11)	−0.0003 (10)
C15	0.0327 (14)	0.0372 (15)	0.0285 (12)	−0.0041 (12)	0.0050 (11)	0.0003 (11)
C16	0.0265 (13)	0.0380 (15)	0.0300 (12)	−0.0045 (11)	0.0028 (10)	0.0000 (11)
C21	0.0307 (14)	0.0350 (14)	0.0293 (12)	−0.0006 (11)	0.0015 (10)	0.0016 (11)
C22	0.0394 (16)	0.0387 (15)	0.0290 (12)	−0.0061 (13)	−0.0005 (11)	0.0064 (11)
C23	0.0361 (15)	0.0362 (15)	0.0307 (13)	−0.0039 (12)	0.0049 (11)	0.0047 (11)
C24	0.0265 (13)	0.0307 (13)	0.0276 (11)	0.0005 (10)	0.0057 (10)	0.0011 (10)
C25	0.0294 (13)	0.0314 (13)	0.0281 (12)	0.0001 (11)	0.0031 (10)	0.0016 (10)
C26	0.0317 (14)	0.0327 (14)	0.0294 (12)	−0.0002 (11)	0.0029 (11)	0.0019 (10)
C27	0.0278 (13)	0.0287 (13)	0.0323 (12)	−0.0012 (10)	0.0075 (10)	−0.0022 (10)
C28	0.0261 (13)	0.0349 (14)	0.0304 (12)	0.0003 (11)	0.0034 (10)	−0.0023 (10)
C29	0.0333 (15)	0.0382 (15)	0.0286 (12)	0.0014 (12)	0.0001 (11)	0.0022 (11)
C30	0.0317 (15)	0.0343 (14)	0.0296 (12)	−0.0037 (11)	0.0020 (11)	0.0035 (11)
O31	0.0328 (11)	0.0473 (13)	0.0309 (10)	−0.0074 (10)	−0.0026 (8)	0.0008 (9)
C31	0.0358 (17)	0.058 (2)	0.0304 (14)	−0.0039 (15)	−0.0031 (12)	0.0013 (13)

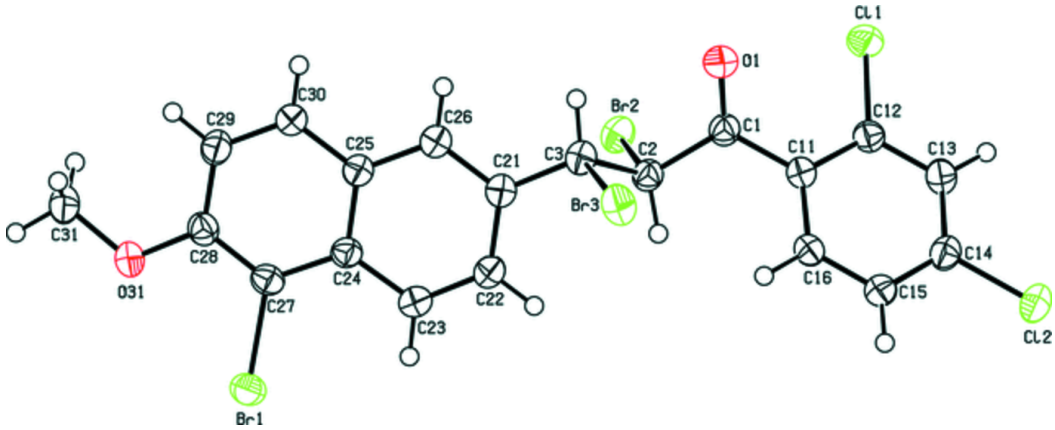
Geometric parameters (Å, °)

O1—C1	1.216 (4)	C21—C26	1.380 (4)
Cl1—C12	1.737 (3)	C21—C22	1.420 (4)
Cl2—C14	1.742 (3)	C22—C23	1.363 (4)
Br1—C27	1.903 (3)	C22—H22	0.9500
Br2—C2	1.973 (3)	C23—C24	1.427 (4)
Br3—C3	2.002 (3)	C23—H23	0.9500
C1—C11	1.492 (4)	C24—C27	1.420 (4)
C1—C2	1.541 (4)	C24—C25	1.432 (4)

C2—C3	1.517 (4)	C25—C26	1.414 (4)
C2—H2	1.0000	C25—C30	1.414 (4)
C3—C21	1.493 (4)	C26—H26	0.9500
C3—H3	1.0000	C27—C28	1.383 (4)
C11—C16	1.399 (4)	C28—O31	1.364 (4)
C11—C12	1.403 (4)	C28—C29	1.421 (4)
C12—C13	1.397 (4)	C29—C30	1.367 (4)
C13—C14	1.385 (4)	C29—H29	0.9500
C13—H13	0.9500	C30—H30	0.9500
C14—C15	1.382 (4)	O31—C31	1.436 (4)
C15—C16	1.382 (4)	C31—H31A	0.9800
C15—H15	0.9500	C31—H31B	0.9800
C16—H16	0.9500	C31—H31C	0.9800
O1—C1—C11	122.9 (3)	C22—C21—C3	122.1 (3)
O1—C1—C2	119.6 (3)	C23—C22—C21	121.2 (3)
C11—C1—C2	117.5 (2)	C23—C22—H22	119.4
C3—C2—C1	112.7 (2)	C21—C22—H22	119.4
C3—C2—Br2	108.74 (18)	C22—C23—C24	121.3 (3)
C1—C2—Br2	103.92 (18)	C22—C23—H23	119.4
C3—C2—H2	110.4	C24—C23—H23	119.4
C1—C2—H2	110.4	C27—C24—C23	124.5 (3)
Br2—C2—H2	110.4	C27—C24—C25	117.9 (2)
C21—C3—C2	117.6 (3)	C23—C24—C25	117.6 (3)
C21—C3—Br3	108.7 (2)	C26—C25—C30	121.3 (3)
C2—C3—Br3	103.93 (18)	C26—C25—C24	119.7 (2)
C21—C3—H3	108.7	C30—C25—C24	119.1 (3)
C2—C3—H3	108.7	C21—C26—C25	121.3 (3)
Br3—C3—H3	108.7	C21—C26—H26	119.3
C16—C11—C12	117.6 (3)	C25—C26—H26	119.3
C16—C11—C1	119.5 (3)	C28—C27—C24	122.1 (3)
C12—C11—C1	122.8 (2)	C28—C27—Br1	118.1 (2)
C13—C12—C11	121.3 (3)	C24—C27—Br1	119.8 (2)
C13—C12—Cl1	117.2 (2)	O31—C28—C27	118.3 (3)
C11—C12—Cl1	121.4 (2)	O31—C28—C29	122.8 (3)
C14—C13—C12	118.3 (3)	C27—C28—C29	119.0 (3)
C14—C13—H13	120.8	C30—C29—C28	120.4 (3)
C12—C13—H13	120.8	C30—C29—H29	119.8
C15—C14—C13	122.2 (3)	C28—C29—H29	119.8
C15—C14—Cl2	118.9 (2)	C29—C30—C25	121.5 (3)
C13—C14—Cl2	118.9 (2)	C29—C30—H30	119.2
C16—C15—C14	118.4 (3)	C25—C30—H30	119.2
C16—C15—H15	120.8	C28—O31—C31	117.1 (2)
C14—C15—H15	120.8	O31—C31—H31A	109.5
C15—C16—C11	122.2 (3)	O31—C31—H31B	109.5
C15—C16—H16	118.9	H31A—C31—H31B	109.5
C11—C16—H16	118.9	O31—C31—H31C	109.5
C26—C21—C22	118.9 (3)	H31A—C31—H31C	109.5
C26—C21—C3	119.0 (3)	H31B—C31—H31C	109.5

O1—C1—C2—C3	−38.8 (4)	C26—C21—C22—C23	−2.2 (5)
C11—C1—C2—C3	141.1 (3)	C3—C21—C22—C23	176.4 (3)
O1—C1—C2—Br2	78.7 (3)	C21—C22—C23—C24	0.9 (5)
C11—C1—C2—Br2	−101.3 (2)	C22—C23—C24—C27	−179.1 (3)
C1—C2—C3—C21	173.0 (2)	C22—C23—C24—C25	0.7 (5)
Br2—C2—C3—C21	58.4 (3)	C27—C24—C25—C26	178.6 (3)
C1—C2—C3—Br3	−66.8 (2)	C23—C24—C25—C26	−1.1 (4)
Br2—C2—C3—Br3	178.53 (13)	C27—C24—C25—C30	−1.5 (4)
O1—C1—C11—C16	134.0 (3)	C23—C24—C25—C30	178.7 (3)
C2—C1—C11—C16	−46.0 (4)	C22—C21—C26—C25	1.7 (5)
O1—C1—C11—C12	−41.1 (4)	C3—C21—C26—C25	−176.9 (3)
C2—C1—C11—C12	138.9 (3)	C30—C25—C26—C21	−179.9 (3)
C16—C11—C12—C13	1.1 (4)	C24—C25—C26—C21	−0.1 (5)
C1—C11—C12—C13	176.3 (3)	C23—C24—C27—C28	−177.9 (3)
C16—C11—C12—Cl1	178.4 (2)	C25—C24—C27—C28	2.4 (4)
C1—C11—C12—Cl1	−6.4 (4)	C23—C24—C27—Br1	3.1 (4)
C11—C12—C13—C14	−2.0 (4)	C25—C24—C27—Br1	−176.7 (2)
Cl1—C12—C13—C14	−179.5 (2)	C24—C27—C28—O31	177.2 (3)
C12—C13—C14—C15	1.4 (5)	Br1—C27—C28—O31	−3.8 (4)
C12—C13—C14—Cl2	−178.9 (2)	C24—C27—C28—C29	−1.9 (4)
C13—C14—C15—C16	0.1 (5)	Br1—C27—C28—C29	177.2 (2)
Cl2—C14—C15—C16	−179.6 (2)	O31—C28—C29—C30	−178.5 (3)
C14—C15—C16—C11	−1.1 (5)	C27—C28—C29—C30	0.5 (5)
C12—C11—C16—C15	0.5 (5)	C28—C29—C30—C25	0.3 (5)
C1—C11—C16—C15	−174.8 (3)	C26—C25—C30—C29	−179.9 (3)
C2—C3—C21—C26	−131.5 (3)	C24—C25—C30—C29	0.2 (5)
Br3—C3—C21—C26	110.8 (3)	C27—C28—O31—C31	−176.7 (3)
C2—C3—C21—C22	50.0 (4)	C29—C28—O31—C31	2.3 (4)
Br3—C3—C21—C22	−67.7 (3)		

Fig. 1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