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(Biphenyl-2-yl)bromidobis(2-methyltetrahydrofuran-κO)magnesium(II)

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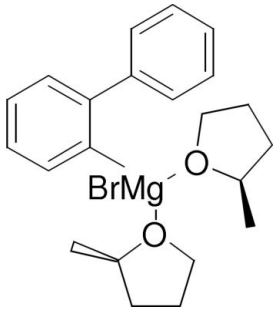
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.007 Å; R factor = 0.045; wR factor = 0.108; data-to-parameter ratio = 17.4.

In the title Grignard reagent, $[MgBr(C_{12}H_9)(C_5H_{10}O)_2]$, the Mg centre adopts a distorted tetrahedral $MgCO_2Br$ arrangement. The dihedral angle between the two aromatic rings of the biphenyl residue is 44.00 (14)°. Each molecule incorporates one *R*- and one *S*-configured 2-methyltetrahydrofuran molecule.

Related literature

For background to Grignard-type compounds, see Elschenbroich (2008); Schwetlick (1996); Silverman & Rakita (1996).



Experimental

Crystal data

$[MgBr(C_{12}H_9)(C_5H_{10}O)_2]$ M_r = 429.67
Monoclinic, $P2_1/n$
a = 11.6887 (5) Å
b = 16.8061 (9) Å
c = 11.7888 (5) Å
β = 103.757 (4)°
V = 2249.38 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.87 mm^{-1}
T = 173 K
0.29 × 0.28 × 0.26 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.614, T_{max} = 0.642
54470 measured reflections
4107 independent reflections
3484 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.108
S = 1.05
4107 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mg1—O1	2.022 (2)	Mg1—C21	2.143 (3)
Mg1—O11	2.030 (2)	Mg1—Br1	2.4750 (10)
O1—Mg1—O11	97.02 (10)	O1—Mg1—Br1	109.97 (9)
O1—Mg1—C21	114.41 (11)	O11—Mg1—Br1	104.75 (7)
O11—Mg1—C21	106.87 (11)	C21—Mg1—Br1	120.53 (8)

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2933).

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supplementary materials

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(Biphenyl-2-yl)bromidobis(2-methyltetrahydrofuran-*κO*)magnesium(II)

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Comment

The title compound is a Grignard reagent, a kind of compounds which is widely used for C—C bond formation or as base in organic chemistry. The Mg centre is four coordinate in a distorted tetrahedral fashion. The bond angles range from 97.02 (1)° for O—Mg—O to 120.53 (8)° for C—Mg—Br. The bond lengths are 2.4750 (10)Å for Mg—Br, 2.143 (3)Å for Mg—C and 2.022 (2)° and 2.030 (2)Å for the Mg—O bonds. The dihedral angles between the two aromatic rings of the biphenyl residue is 44.00 (14)°.

Experimental

This compound is commercially available from Chemetall GmbH (CAS 82214–69-5, Product No. 408562). Colourless blocks of (I) were obtained from a solution due to long term storage at ambient temperature.

Refinement

The H atoms bonded were geometrically positioned and refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C) or U(H) = 1.5 U_{eq}(C_{methyl})] using a riding model with $C_{aromatic}$—H = 0.95 Å, C_{methyl}—H = 0.98 Å, $C_{methylene}$—H = 0.99Å and $C_{tertiary}$—H = 1.00 Å.

Figures

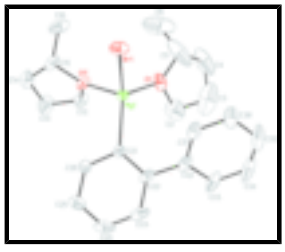


Fig. 1. Perspective view of (I) with displacement ellipsoids drawn at the 50% probability level; H atoms omitted for clarity.

(Biphenyl-2-yl)bromidobis(2-methyltetrahydrofuran-κ*O*)magnesium(II)

Crystal data

$[MgBr(C_{12}H_9)(C_5H_{10}O)_2]$	F_{000} = 896
M_r = 429.67	D_x = 1.269 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 40381 reflections
a = 11.6887 (5) Å	θ = 3.6–26.6°

b = 16.8061 (9) Å	μ = 1.87 mm^{-1}
c = 11.7888 (5) Å	T = 173 K
β = 103.757 (4)º	Block, colourless
V = 2249.38 (18) Å^3	0.29 × 0.28 × 0.26 mm
Z = 4	

Data collection

Stoe IPDSII two-circle diffractometer	4107 independent reflections
Radiation source: fine-focus sealed tube	3484 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.069
T = 173 K	θ_{max} = 25.4º
ω scans	θ_{min} = 3.6º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	h = −14→14
T_{min} = 0.614, T_{max} = 0.642	k = −20→20
54470 measured reflections	l = −14→14

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 2.3133P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.108	$(\Delta/\sigma)_{max} < 0.001$
S = 1.05	$\Delta\rho_{max}$ = 0.76 e Å^{-3}
4107 reflections	$\Delta\rho_{min}$ = −0.41 e Å^{-3}
236 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0043 (6)
Secondary atom site location: difference Fourier map	

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 $F^2 > \sigma(F^2)$ 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}
Mg1	0.56815 (8)	0.31486 (6)	0.70780 (8)	0.0349 (2)
Br1	0.60093 (3)	0.24360 (2)	0.89652 (3)	0.05398 (15)
O1	0.4214 (2)	0.38260 (15)	0.6841 (2)	0.0572 (6)
C2	0.4112 (4)	0.4578 (4)	0.6045 (5)	0.0967 (17)
H2A	0.4898	0.4781	0.6011	0.116*
H2B	0.3649	0.4465	0.5243	0.116*
C3	0.3515 (7)	0.5122 (4)	0.6625 (8)	0.159 (4)
H3A	0.3114	0.5542	0.6085	0.190*
H3B	0.4067	0.5376	0.7296	0.190*
C4	0.2618 (6)	0.4595 (5)	0.7036 (7)	0.145 (3)
H4A	0.2312	0.4860	0.7653	0.173*
H4B	0.1951	0.4450	0.6379	0.173*
C5	0.3367 (5)	0.3866 (6)	0.7512 (5)	0.143 (3)
H5	0.3763	0.3948	0.8354	0.172*
C6	0.2702 (6)	0.3147 (6)	0.7372 (7)	0.170 (4)
H6A	0.3212	0.2705	0.7720	0.256*
H6B	0.2383	0.3044	0.6539	0.256*
H6C	0.2052	0.3199	0.7762	0.256*
O11	0.50159 (19)	0.23129 (11)	0.58553 (18)	0.0412 (5)
C12	0.4587 (3)	0.2531 (2)	0.4632 (3)	0.0536 (8)
H12A	0.4940	0.3040	0.4464	0.064*
H12B	0.3718	0.2587	0.4430	0.064*
C13	0.4955 (5)	0.1870 (3)	0.3968 (4)	0.0852 (15)
H13A	0.4355	0.1777	0.3231	0.102*
H13B	0.5713	0.1998	0.3774	0.102*
C14	0.5080 (4)	0.1158 (2)	0.4719 (4)	0.0672 (11)
H14A	0.5833	0.0884	0.4732	0.081*
H14B	0.4426	0.0782	0.4422	0.081*
C15	0.5056 (3)	0.14444 (18)	0.5944 (3)	0.0521 (9)
H15	0.5799	0.1279	0.6508	0.063*
C16	0.4023 (4)	0.1148 (3)	0.6359 (4)	0.0790 (13)
H16A	0.4065	0.1351	0.7147	0.119*
H16B	0.4032	0.0565	0.6373	0.119*
H16C	0.3294	0.1334	0.5829	0.119*
C21	0.7121 (2)	0.37048 (16)	0.6550 (2)	0.0341 (6)
C22	0.7636 (2)	0.44648 (17)	0.6866 (3)	0.0395 (7)
C23	0.8611 (3)	0.4719 (2)	0.6460 (3)	0.0549 (9)
H23	0.8928	0.5234	0.6666	0.066*
C24	0.9121 (3)	0.4234 (3)	0.5767 (4)	0.0627 (11)
H24	0.9794	0.4411	0.5518	0.075*
C25	0.8648 (3)	0.3495 (2)	0.5439 (3)	0.0542 (9)
H25	0.8986	0.3159	0.4959	0.065*
C26	0.7668 (3)	0.32490 (18)	0.5821 (3)	0.0419 (7)
H26	0.7345	0.2741	0.5577	0.050*
C31	0.6804 (3)	0.4711 (2)	0.8611 (3)	0.0483 (8)

H31	0.6914	0.4163	0.8802	0.058*
C32	0.7136 (3)	0.50025 (17)	0.7624 (3)	0.0442 (8)
C33	0.6971 (4)	0.5819 (2)	0.7384 (3)	0.0638 (11)
H33	0.7205	0.6039	0.6732	0.077*
C34	0.6474 (5)	0.6307 (2)	0.8081 (4)	0.0854 (16)
H34	0.6354	0.6855	0.7890	0.102*
C35	0.6154 (4)	0.6014 (3)	0.9041 (4)	0.0853 (16)
H35	0.5821	0.6356	0.9517	0.102*
C36	0.6318 (4)	0.5206 (2)	0.9319 (3)	0.0656 (11)
H36	0.6099	0.4997	0.9986	0.079*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0308 (5)	0.0364 (5)	0.0377 (5)	−0.0051 (4)	0.0085 (4)	−0.0023 (4)
Br1	0.0496 (2)	0.0716 (3)	0.0401 (2)	−0.01271 (17)	0.00923 (14)	0.00894 (16)
O1	0.0412 (13)	0.0673 (16)	0.0586 (15)	0.0132 (11)	0.0029 (11)	−0.0154 (12)
C2	0.059 (3)	0.116 (4)	0.106 (4)	0.027 (3)	0.002 (3)	0.014 (3)
C3	0.129 (6)	0.114 (5)	0.174 (8)	0.051 (5)	−0.082 (6)	−0.039 (5)
C4	0.103 (5)	0.204 (8)	0.133 (6)	0.102 (6)	0.039 (4)	−0.001 (5)
C5	0.080 (4)	0.269 (10)	0.082 (4)	0.081 (5)	0.023 (3)	−0.001 (5)
C6	0.086 (5)	0.277 (12)	0.145 (7)	−0.072 (6)	0.022 (4)	0.027 (7)
O11	0.0477 (12)	0.0308 (11)	0.0408 (11)	−0.0064 (9)	0.0017 (9)	0.0021 (8)
C12	0.065 (2)	0.0477 (19)	0.0407 (17)	−0.0002 (17)	−0.0019 (15)	0.0043 (15)
C13	0.137 (5)	0.065 (3)	0.054 (2)	−0.002 (3)	0.024 (3)	−0.013 (2)
C14	0.072 (3)	0.050 (2)	0.075 (3)	0.0072 (19)	0.009 (2)	−0.0172 (19)
C15	0.054 (2)	0.0317 (16)	0.061 (2)	−0.0068 (14)	−0.0061 (16)	0.0057 (15)
C16	0.090 (3)	0.069 (3)	0.073 (3)	−0.043 (2)	0.010 (2)	0.003 (2)
C21	0.0299 (13)	0.0292 (14)	0.0409 (15)	0.0013 (11)	0.0038 (11)	0.0036 (12)
C22	0.0312 (14)	0.0343 (15)	0.0451 (17)	−0.0061 (12)	−0.0063 (12)	0.0082 (13)
C23	0.0436 (19)	0.054 (2)	0.058 (2)	−0.0204 (16)	−0.0055 (16)	0.0150 (17)
C24	0.0345 (17)	0.086 (3)	0.067 (2)	−0.0100 (18)	0.0113 (16)	0.025 (2)
C25	0.0435 (18)	0.066 (2)	0.057 (2)	0.0104 (17)	0.0198 (16)	0.0174 (18)
C26	0.0397 (16)	0.0364 (16)	0.0507 (18)	0.0063 (13)	0.0129 (14)	0.0064 (13)
C31	0.0481 (18)	0.0392 (17)	0.0478 (19)	0.0046 (14)	−0.0079 (14)	−0.0072 (14)
C32	0.0417 (16)	0.0341 (16)	0.0450 (18)	−0.0045 (13)	−0.0132 (13)	−0.0052 (13)
C33	0.082 (3)	0.0333 (18)	0.055 (2)	−0.0038 (17)	−0.0242 (19)	−0.0040 (16)
C34	0.124 (4)	0.038 (2)	0.065 (3)	0.015 (2)	−0.035 (3)	−0.017 (2)
C35	0.103 (4)	0.064 (3)	0.066 (3)	0.033 (2)	−0.025 (3)	−0.034 (2)
C36	0.069 (2)	0.068 (2)	0.049 (2)	0.013 (2)	−0.0076 (18)	−0.0172 (18)

Geometric parameters (Å, °)

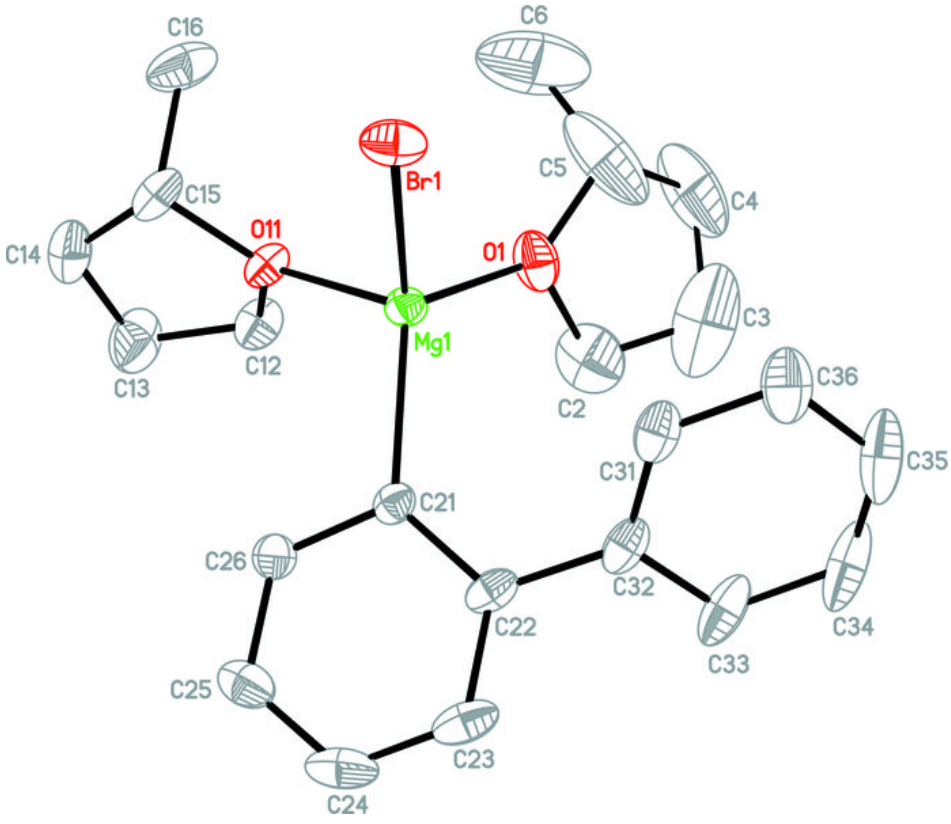
Mg1—O1	2.022 (2)	C14—H14A	0.9900
Mg1—O11	2.030 (2)	C14—H14B	0.9900
Mg1—C21	2.143 (3)	C15—C16	1.492 (5)
Mg1—Br1	2.4750 (10)	C15—H15	1.0000
O1—C5	1.408 (6)	C16—H16A	0.9800
O1—C2	1.562 (6)	C16—H16B	0.9800

C2—C3	1.421 (9)	C16—H16C	0.9800
C2—H2A	0.9900	C21—C26	1.412 (4)
C2—H2B	0.9900	C21—C22	1.424 (4)
C3—C4	1.536 (11)	C22—C23	1.403 (5)
C3—H3A	0.9900	C22—C32	1.485 (5)
C3—H3B	0.9900	C23—C24	1.385 (6)
C4—C5	1.533 (9)	C23—H23	0.9500
C4—H4A	0.9900	C24—C25	1.377 (6)
C4—H4B	0.9900	C24—H24	0.9500
C5—C6	1.425 (11)	C25—C26	1.390 (4)
C5—H5	1.0000	C25—H25	0.9500
C6—H6A	0.9800	C26—H26	0.9500
C6—H6B	0.9800	C31—C36	1.393 (5)
C6—H6C	0.9800	C31—C32	1.399 (5)
O11—C12	1.456 (4)	C31—H31	0.9500
O11—C15	1.463 (4)	C32—C33	1.404 (4)
C12—C13	1.481 (5)	C33—C34	1.384 (6)
C12—H12A	0.9900	C33—H33	0.9500
C12—H12B	0.9900	C34—C35	1.366 (7)
C13—C14	1.475 (6)	C34—H34	0.9500
C13—H13A	0.9900	C35—C36	1.398 (6)
C13—H13B	0.9900	C35—H35	0.9500
C14—C15	1.529 (5)	C36—H36	0.9500
O1—Mg1—O11	97.02 (10)	C13—C14—C15	106.8 (3)
O1—Mg1—C21	114.41 (11)	C13—C14—H14A	110.4
O11—Mg1—C21	106.87 (11)	C15—C14—H14A	110.4
O1—Mg1—Br1	109.97 (9)	C13—C14—H14B	110.4
O11—Mg1—Br1	104.75 (7)	C15—C14—H14B	110.4
C21—Mg1—Br1	120.53 (8)	H14A—C14—H14B	108.6
C5—O1—C2	109.6 (4)	O11—C15—C16	110.0 (3)
C5—O1—Mg1	129.5 (3)	O11—C15—C14	104.7 (3)
C2—O1—Mg1	118.7 (2)	C16—C15—C14	113.8 (3)
C3—C2—O1	102.0 (5)	O11—C15—H15	109.4
C3—C2—H2A	111.4	C16—C15—H15	109.4
O1—C2—H2A	111.4	C14—C15—H15	109.4
C3—C2—H2B	111.4	C15—C16—H16A	109.5
O1—C2—H2B	111.4	C15—C16—H16B	109.5
H2A—C2—H2B	109.2	H16A—C16—H16B	109.5
C2—C3—C4	103.3 (6)	C15—C16—H16C	109.5
C2—C3—H3A	111.1	H16A—C16—H16C	109.5
C4—C3—H3A	111.1	H16B—C16—H16C	109.5
C2—C3—H3B	111.1	C26—C21—C22	114.9 (3)
C4—C3—H3B	111.1	C26—C21—Mg1	116.1 (2)
H3A—C3—H3B	109.1	C22—C21—Mg1	128.9 (2)
C5—C4—C3	101.7 (5)	C23—C22—C21	120.8 (3)
C5—C4—H4A	111.4	C23—C22—C32	119.2 (3)
C3—C4—H4A	111.4	C21—C22—C32	120.0 (3)
C5—C4—H4B	111.4	C24—C23—C22	121.3 (3)
C3—C4—H4B	111.4	C24—C23—H23	119.3

H4A—C4—H4B	109.3	C22—C23—H23	119.3
O1—C5—C6	109.4 (6)	C25—C24—C23	119.7 (3)
O1—C5—C4	104.4 (6)	C25—C24—H24	120.1
C6—C5—C4	112.8 (7)	C23—C24—H24	120.1
O1—C5—H5	110.0	C24—C25—C26	119.0 (3)
C6—C5—H5	110.0	C24—C25—H25	120.5
C4—C5—H5	110.0	C26—C25—H25	120.5
C5—C6—H6A	109.5	C25—C26—C21	124.2 (3)
C5—C6—H6B	109.5	C25—C26—H26	117.9
H6A—C6—H6B	109.5	C21—C26—H26	117.9
C5—C6—H6C	109.5	C36—C31—C32	121.6 (3)
H6A—C6—H6C	109.5	C36—C31—H31	119.2
H6B—C6—H6C	109.5	C32—C31—H31	119.2
C12—O11—C15	108.6 (2)	C31—C32—C33	117.2 (3)
C12—O11—Mg1	120.80 (18)	C31—C32—C22	121.0 (3)
C15—O11—Mg1	129.73 (19)	C33—C32—C22	121.8 (3)
O11—C12—C13	105.0 (3)	C34—C33—C32	121.1 (4)
O11—C12—H12A	110.7	C34—C33—H33	119.5
C13—C12—H12A	110.7	C32—C33—H33	119.5
O11—C12—H12B	110.7	C35—C34—C33	121.0 (4)
C13—C12—H12B	110.7	C35—C34—H34	119.5
H12A—C12—H12B	108.8	C33—C34—H34	119.5
C14—C13—C12	106.9 (3)	C34—C35—C36	119.7 (4)
C14—C13—H13A	110.3	C34—C35—H35	120.1
C12—C13—H13A	110.3	C36—C35—H35	120.1
C14—C13—H13B	110.3	C31—C36—C35	119.4 (4)
C12—C13—H13B	110.3	C31—C36—H36	120.3
H13A—C13—H13B	108.6	C35—C36—H36	120.3
O11—Mg1—O1—C5	101.5 (5)	C13—C14—C15—C16	115.6 (4)
C21—Mg1—O1—C5	−146.4 (5)	O1—Mg1—C21—C26	−130.5 (2)
Br1—Mg1—O1—C5	−7.1 (5)	O11—Mg1—C21—C26	−24.4 (2)
O11—Mg1—O1—C2	−97.5 (3)	Br1—Mg1—C21—C26	94.8 (2)
C21—Mg1—O1—C2	14.7 (3)	O1—Mg1—C21—C22	52.0 (3)
Br1—Mg1—O1—C2	154.0 (3)	O11—Mg1—C21—C22	158.2 (2)
C5—O1—C2—C3	20.6 (6)	Br1—Mg1—C21—C22	−82.6 (3)
Mg1—O1—C2—C3	−144.0 (4)	C26—C21—C22—C23	0.3 (4)
O1—C2—C3—C4	−38.6 (5)	Mg1—C21—C22—C23	177.7 (2)
C2—C3—C4—C5	43.7 (7)	C26—C21—C22—C32	179.6 (3)
C2—O1—C5—C6	127.7 (6)	Mg1—C21—C22—C32	−2.9 (4)
Mg1—O1—C5—C6	−69.9 (7)	C21—C22—C23—C24	−1.6 (5)
C2—O1—C5—C4	6.8 (7)	C32—C22—C23—C24	179.0 (3)
Mg1—O1—C5—C4	169.2 (4)	C22—C23—C24—C25	1.7 (5)
C3—C4—C5—O1	−29.7 (8)	C23—C24—C25—C26	−0.4 (5)
C3—C4—C5—C6	−148.4 (7)	C24—C25—C26—C21	−1.0 (5)
O1—Mg1—O11—C12	60.3 (3)	C22—C21—C26—C25	1.1 (4)
C21—Mg1—O11—C12	−57.9 (3)	Mg1—C21—C26—C25	−176.7 (2)
Br1—Mg1—O11—C12	173.1 (2)	C36—C31—C32—C33	0.8 (5)
O1—Mg1—O11—C15	−131.4 (3)	C36—C31—C32—C22	−179.0 (3)
C21—Mg1—O11—C15	110.4 (3)	C23—C22—C32—C31	−136.9 (3)

Br1—Mg1—O11—C15	−18.6 (3)	C21—C22—C32—C31	43.7 (4)
C15—O11—C12—C13	−28.8 (4)	C23—C22—C32—C33	43.3 (4)
Mg1—O11—C12—C13	141.7 (3)	C21—C22—C32—C33	−136.1 (3)
O11—C12—C13—C14	25.2 (5)	C31—C32—C33—C34	−1.6 (5)
C12—C13—C14—C15	−12.7 (5)	C22—C32—C33—C34	178.2 (3)
C12—O11—C15—C16	−102.0 (3)	C32—C33—C34—C35	1.6 (6)
Mg1—O11—C15—C16	88.6 (3)	C33—C34—C35—C36	−0.7 (7)
C12—O11—C15—C14	20.7 (4)	C32—C31—C36—C35	0.1 (5)
Mg1—O11—C15—C14	−148.7 (2)	C34—C35—C36—C31	−0.1 (6)
C13—C14—C15—O11	−4.6 (4)		

Fig. 1


C16
C6
Br1
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