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(*R*)-3,3′-Bis(3,4,5-trifluorophenyl)-1,1′-binaphthalene-2,2′-diol

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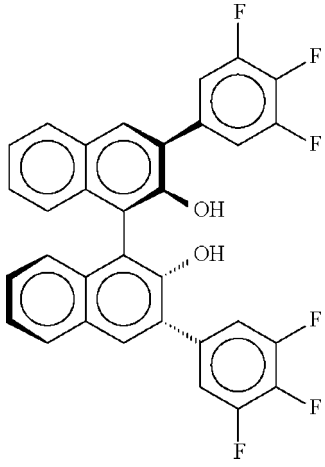
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.012 Å; R factor = 0.070; wR factor = 0.184; data-to-parameter ratio = 6.6.

The two fused-ring systems in the title molecule, $C_{32}H_{16}F_6O_2$, are twisted by 73.5 (1)° about the central C—C single bond, thereby conferring chirality on the molecule.

Related literature

For the synthesis of the compound, see: Kano *et al.* (2006). For related literature, see: He & Ng (2006, 2007).



Experimental

Crystal data

$C_{32}H_{16}F_2O_2$
M_r = 546.45
Monoclinic, $P2_1$
a = 12.440 (4) Å
b = 7.466 (3) Å
c = 14.443 (5) Å
β = 111.22 (3)°
V = 1250.5 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 295 (2) K
0.25 × 0.25 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
2385 measured reflections
2378 independent reflections
1302 reflections with $I > 2\sigma(I)$
R_{int} = 0.006
3 standard reflections
frequency: 60 min
intensity decay: 3.6%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.184
S = 1.08
2378 reflections
362 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Data collection: *DIFRAC* (Gabe *et al.*, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2424).

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supplementary materials

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(*R*)-3,3'-Bis(3,4,5-trifluorophenyl)-1,1'-binaphthalene-2,2'-diol

T.-R. Kang, L. He and S. W. Ng

Comment

We have reported two chiral, substituted BINOL [(1,1'-binaphthalene-2,2'-diol] derivatives recently (He & Ng, 2006, 2007). Our studies continue with the crystal structure determinarion of title compound. A tin(IV) derivative is a chiral tin alkoxide this is an efficient Lewis-acidic catalyst for enantionselective Diels-Alder reactions (Kano *et al.*, 2006). In the title molecule the two fused-rings are twisted along the central carbon–carbon single bond that confers chirality to the molecule by 73.5 (1) °. The two hydroxy groups do not engage in any hydrogen bonding interactions.

Experimental

The chiral compound was synthesized by the procedure of Kano *et al.* (2006), and crystals were grown from its solution in ethanol. However, the starting BINOL [(1,1'-binaphthalene-2,2'-diol] had an *R*- instead of an *S*-configuration. Methylation of (*R*)-1,1'-binaphthalene-2,2'-diol with methyl iodide gave dimethoxybinaphthyl; this was treated with *n*-butyl lithium and *N*,*N*,*N*',*N*'-tetramethylenediamine in ether at room temperature to give the dilithiated compound, which was brominated at 195 K to afford the dibromide. The dibromide was coupled with 3,4,5-trifluorophenylmagnesium bromide in the presence of commercially available dichlorobis(triphenylphosphinenickel as a catalyst; the product was demethylated to give the title compound.

Refinement

In the absence of significant anomalous dispersion effects Friedel pairs were merged. The *R*-configuration was selected on the basis of the starting material. The oxygen- and carbon-bound H-atoms were generated geometrically (O—H 0.82 Å and C—H 0.93 Å), and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 to 1.5U_{eq}(C,*O*).

The configuration selected is the *R*-enantiomer.

Figures

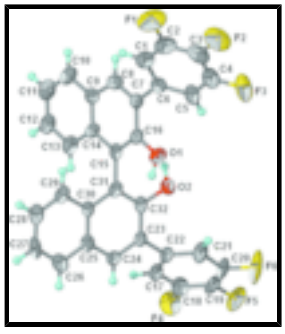


Fig. 1. The molecular structure with displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius.

(*R*)-3,3'-Bis(3,4,5-trifluorophenyl)-1,1'-binaphthalene-2,2'-diol

Crystal data

$C_{32}H_{16}F_2O_2$	F_{000} = 556
M_r = 546.45	D_x = 1.451 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 24 reflections
a = 12.440 (4) Å	θ = 4.9–7.5º
b = 7.466 (3) Å	μ = 0.12 mm^{-1}
c = 14.443 (5) Å	T = 295 (2) K
β = 111.22 (3)º	Block, colourless
V = 1250.5 (8) Å^3	0.25 × 0.25 × 0.18 mm
Z = 2	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.006
Radiation source: medium-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 1.5º
T = 295(2) K	h = −14→13
$\omega/2\theta$ scans	k = −1→8
Absorption correction: none	l = −4→17
2385 measured reflections	3 standard reflections
2378 independent reflections	every 60 min
1302 reflections with $I > 2\sigma(I)$	intensity decay: 3.6%

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.070	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.184	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
S = 1.08	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
2378 reflections	Extinction correction: none
362 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.2343 (5)	0.5000 (12)	0.5656 (5)	0.123 (3)
F2	0.1556 (5)	0.8419 (9)	0.5493 (5)	0.115 (2)
F3	−0.0080 (6)	0.9311 (7)	0.6199 (4)	0.0989 (19)
F4	−0.6890 (5)	0.2983 (9)	0.9932 (4)	0.097 (2)
F5	−0.6902 (5)	0.6582 (9)	0.9799 (4)	0.101 (2)
F6	−0.5947 (8)	0.8181 (8)	0.8609 (6)	0.131 (3)
O1	−0.2115 (4)	0.4216 (7)	0.6543 (4)	0.0578 (15)
H1O	−0.2775	0.3822	0.6356	0.069*
O2	−0.3059 (4)	0.4018 (7)	0.8444 (4)	0.0584 (15)
H2O	−0.2366	0.3935	0.8555	0.070*
C1	0.1105 (6)	0.4153 (12)	0.6469 (6)	0.064 (2)
H1	0.1385	0.2988	0.6516	0.077*
C2	0.1510 (7)	0.5459 (16)	0.6029 (7)	0.074 (3)
C3	0.1132 (8)	0.7189 (15)	0.5942 (7)	0.075 (3)
C4	0.0327 (8)	0.7594 (13)	0.6315 (6)	0.068 (2)
C5	−0.0149 (8)	0.6364 (11)	0.6768 (6)	0.060 (2)
H5	−0.0718	0.6696	0.7011	0.072*
C6	0.0253 (6)	0.4612 (11)	0.6849 (5)	0.0474 (19)
C7	−0.0189 (6)	0.3195 (10)	0.7359 (5)	0.0442 (18)
C8	0.0531 (6)	0.1995 (11)	0.7967 (6)	0.052 (2)
H8	0.1318	0.2124	0.8104	0.062*
C9	0.0159 (6)	0.0541 (11)	0.8412 (5)	0.0443 (17)
C10	0.0923 (7)	−0.0752 (13)	0.9012 (6)	0.063 (2)
H10	0.1708	−0.0670	0.9130	0.075*
C11	0.0526 (7)	−0.2098 (13)	0.9413 (5)	0.065 (2)
H11	0.1041	−0.2950	0.9797	0.078*
C12	−0.0626 (7)	−0.2249 (12)	0.9269 (6)	0.061 (2)
H12	−0.0876	−0.3196	0.9559	0.073*
C13	−0.1411 (7)	−0.1022 (11)	0.8704 (5)	0.054 (2)
H13	−0.2186	−0.1116	0.8621	0.065*
C14	−0.1022 (6)	0.0399 (10)	0.8245 (5)	0.0428 (17)
C15	−0.1812 (6)	0.1692 (9)	0.7612 (5)	0.0404 (17)
C16	−0.1382 (6)	0.3031 (10)	0.7189 (5)	0.0422 (17)
C17	−0.5886 (6)	0.2731 (10)	0.8830 (5)	0.052 (2)
H17	−0.5905	0.1489	0.8867	0.062*
C18	−0.6390 (7)	0.3785 (12)	0.9343 (6)	0.066 (3)
C19	−0.6397 (7)	0.5568 (14)	0.9287 (6)	0.066 (2)
C20	−0.5907 (9)	0.6369 (11)	0.8695 (7)	0.068 (3)
C21	−0.5354 (8)	0.5422 (12)	0.8169 (6)	0.065 (2)
H21	−0.5005	0.5998	0.7780	0.079*
C22	−0.5347 (6)	0.3574 (10)	0.8254 (6)	0.0463 (19)
C23	−0.4783 (6)	0.2434 (9)	0.7710 (5)	0.0404 (17)
C24	−0.5403 (6)	0.1043 (9)	0.7110 (5)	0.0428 (18)
H24	−0.6176	0.0883	0.7018	0.051*
C25	−0.4869 (6)	−0.0125 (10)	0.6639 (5)	0.0473 (19)

C26	−0.5508 (7)	−0.1538 (11)	0.6018 (6)	0.060 (2)
H26	−0.6281	−0.1712	0.5923	0.071*
C27	−0.4964 (8)	−0.2639 (11)	0.5564 (6)	0.062 (2)
H27	−0.5373	−0.3586	0.5178	0.075*
C28	−0.3845 (7)	−0.2387 (11)	0.5660 (6)	0.058 (2)
H28	−0.3514	−0.3121	0.5317	0.069*
C29	−0.3209 (7)	−0.1062 (10)	0.6260 (5)	0.0481 (19)
H29	−0.2438	−0.0914	0.6338	0.058*
C30	−0.3717 (6)	0.0087 (9)	0.6763 (5)	0.0382 (16)
C31	−0.3087 (6)	0.1503 (10)	0.7384 (5)	0.0427 (18)
C32	−0.3635 (6)	0.2634 (9)	0.7828 (5)	0.0421 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.096 (4)	0.168 (7)	0.148 (5)	0.013 (5)	0.098 (4)	0.025 (5)
F2	0.117 (4)	0.122 (6)	0.127 (5)	−0.037 (4)	0.071 (4)	0.041 (4)
F3	0.159 (5)	0.050 (3)	0.108 (4)	−0.018 (4)	0.072 (4)	0.010 (3)
F4	0.120 (4)	0.095 (4)	0.123 (4)	−0.013 (4)	0.102 (4)	−0.013 (4)
F5	0.115 (5)	0.092 (4)	0.124 (5)	0.037 (4)	0.076 (4)	−0.027 (4)
F6	0.228 (8)	0.039 (3)	0.168 (6)	0.037 (4)	0.121 (6)	0.002 (4)
O1	0.050 (3)	0.052 (3)	0.083 (4)	0.009 (3)	0.037 (3)	0.029 (3)
O2	0.055 (3)	0.052 (3)	0.080 (3)	−0.007 (3)	0.040 (3)	−0.022 (3)
C1	0.062 (5)	0.069 (6)	0.081 (6)	−0.002 (5)	0.049 (5)	0.005 (5)
C2	0.061 (5)	0.097 (8)	0.088 (6)	0.000 (6)	0.057 (5)	0.001 (6)
C3	0.077 (6)	0.083 (7)	0.076 (6)	−0.030 (6)	0.042 (5)	0.012 (6)
C4	0.085 (6)	0.058 (6)	0.069 (6)	−0.013 (5)	0.039 (5)	0.000 (5)
C5	0.082 (6)	0.044 (5)	0.065 (5)	−0.009 (5)	0.041 (5)	−0.001 (4)
C6	0.050 (4)	0.052 (5)	0.052 (4)	−0.006 (4)	0.032 (4)	−0.007 (4)
C7	0.046 (4)	0.035 (4)	0.062 (5)	−0.002 (4)	0.032 (4)	0.003 (4)
C8	0.047 (4)	0.056 (5)	0.065 (5)	−0.003 (4)	0.034 (4)	−0.002 (4)
C9	0.051 (4)	0.043 (4)	0.041 (4)	−0.002 (4)	0.019 (4)	−0.007 (4)
C10	0.064 (5)	0.062 (6)	0.067 (5)	0.019 (5)	0.031 (5)	0.002 (5)
C11	0.083 (6)	0.059 (5)	0.049 (5)	0.016 (5)	0.020 (5)	0.011 (5)
C12	0.078 (6)	0.046 (5)	0.063 (5)	0.012 (5)	0.031 (5)	0.018 (4)
C13	0.068 (5)	0.051 (5)	0.057 (5)	0.006 (4)	0.039 (4)	0.010 (4)
C14	0.046 (4)	0.043 (4)	0.044 (4)	0.010 (4)	0.023 (3)	0.005 (4)
C15	0.055 (4)	0.033 (4)	0.046 (4)	0.001 (3)	0.033 (4)	−0.001 (3)
C16	0.048 (4)	0.036 (4)	0.050 (4)	0.005 (4)	0.028 (4)	0.001 (4)
C17	0.064 (5)	0.040 (4)	0.070 (5)	0.006 (4)	0.048 (4)	−0.005 (4)
C18	0.078 (6)	0.063 (7)	0.088 (7)	−0.007 (5)	0.067 (6)	−0.012 (5)
C19	0.068 (6)	0.066 (6)	0.075 (6)	0.030 (5)	0.037 (5)	−0.012 (5)
C20	0.087 (7)	0.036 (5)	0.087 (6)	0.023 (5)	0.038 (6)	−0.001 (5)
C21	0.090 (6)	0.046 (5)	0.085 (6)	0.011 (5)	0.060 (5)	0.004 (5)
C22	0.053 (4)	0.038 (4)	0.064 (5)	0.004 (3)	0.040 (4)	−0.005 (4)
C23	0.050 (4)	0.033 (4)	0.047 (4)	0.004 (4)	0.027 (4)	0.000 (4)
C24	0.044 (4)	0.041 (4)	0.055 (4)	0.002 (4)	0.032 (4)	0.002 (4)
C25	0.061 (5)	0.039 (4)	0.051 (4)	0.001 (4)	0.031 (4)	0.002 (4)

C26	0.072 (5)	0.052 (5)	0.062 (5)	−0.013 (4)	0.033 (4)	−0.002 (4)
C27	0.099 (6)	0.032 (4)	0.062 (5)	−0.006 (4)	0.036 (5)	−0.010 (4)
C28	0.083 (6)	0.046 (5)	0.052 (4)	0.004 (5)	0.034 (4)	−0.009 (4)
C29	0.060 (4)	0.049 (5)	0.042 (4)	0.014 (4)	0.027 (4)	0.005 (4)
C30	0.052 (4)	0.031 (4)	0.040 (4)	−0.001 (3)	0.026 (3)	0.001 (3)
C31	0.050 (4)	0.042 (4)	0.045 (4)	0.007 (4)	0.029 (4)	0.003 (4)
C32	0.058 (4)	0.033 (4)	0.044 (4)	−0.001 (4)	0.029 (4)	−0.002 (3)

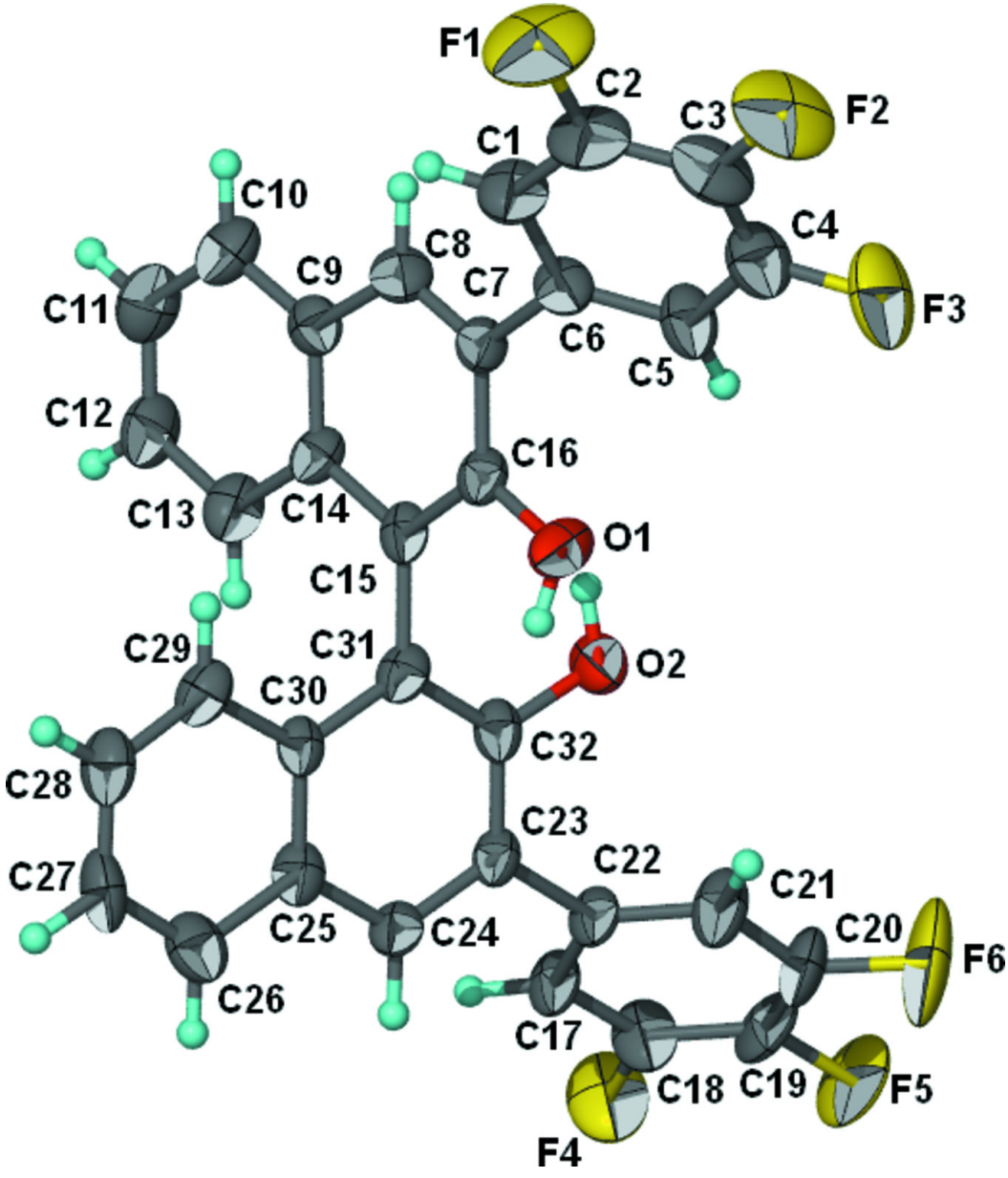
Geometric parameters (Å, °)

F1—C2	1.374 (9)	C13—C14	1.426 (10)
F2—C3	1.337 (10)	C13—H13	0.9300
F3—C4	1.367 (11)	C14—C15	1.442 (10)
F4—C18	1.361 (9)	C15—C16	1.377 (9)
F5—C19	1.361 (9)	C15—C31	1.506 (9)
F6—C20	1.357 (10)	C17—C18	1.378 (10)
O1—C16	1.367 (9)	C17—C22	1.392 (9)
O1—H1O	0.8200	C17—H17	0.9300
O2—C32	1.382 (8)	C18—C19	1.333 (13)
O2—H2O	0.8200	C19—C20	1.355 (12)
C1—C2	1.356 (12)	C20—C21	1.389 (11)
C1—C6	1.402 (9)	C21—C22	1.385 (12)
C1—H1	0.9300	C21—H21	0.9300
C2—C3	1.365 (15)	C22—C23	1.494 (9)
C3—C4	1.332 (12)	C23—C32	1.384 (9)
C4—C5	1.379 (11)	C23—C24	1.393 (9)
C5—C6	1.390 (11)	C24—C25	1.410 (9)
C5—H5	0.9300	C24—H24	0.9300
C6—C7	1.503 (10)	C25—C30	1.388 (9)
C7—C8	1.344 (10)	C25—C26	1.425 (11)
C7—C16	1.420 (9)	C26—C27	1.373 (11)
C8—C9	1.422 (11)	C26—H26	0.9300
C8—H8	0.9300	C27—C28	1.361 (10)
C9—C14	1.405 (9)	C27—H27	0.9300
C9—C10	1.410 (11)	C28—C29	1.364 (10)
C10—C11	1.340 (12)	C28—H28	0.9300
C10—H10	0.9300	C29—C30	1.413 (9)
C11—C12	1.377 (10)	C29—H29	0.9300
C11—H11	0.9300	C30—C31	1.424 (9)
C12—C13	1.372 (10)	C31—C32	1.380 (9)
C12—H12	0.9300		
C16—O1—H1O	109.5	C15—C16—C7	122.4 (7)
C32—O2—H2O	109.5	C18—C17—C22	118.3 (7)
C2—C1—C6	118.0 (8)	C18—C17—H17	120.8
C2—C1—H1	121.0	C22—C17—H17	120.8
C6—C1—H1	121.0	C19—C18—F4	118.9 (8)
C1—C2—C3	123.4 (7)	C19—C18—C17	122.1 (8)
C1—C2—F1	117.7 (10)	F4—C18—C17	119.0 (8)
C3—C2—F1	118.9 (9)	C18—C19—C20	119.0 (7)

C4—C3—F2	121.8 (10)	C18—C19—F5	121.1 (9)
C4—C3—C2	117.5 (8)	C20—C19—F5	119.9 (9)
F2—C3—C2	120.8 (9)	C19—C20—F6	119.2 (8)
C3—C4—F3	117.6 (8)	C19—C20—C21	123.0 (7)
C3—C4—C5	123.8 (9)	F6—C20—C21	117.8 (8)
F3—C4—C5	118.6 (8)	C22—C21—C20	116.5 (8)
C4—C5—C6	117.6 (8)	C22—C21—H21	121.7
C4—C5—H5	121.2	C20—C21—H21	121.7
C6—C5—H5	121.2	C21—C22—C17	121.0 (7)
C5—C6—C1	119.8 (7)	C21—C22—C23	120.6 (6)
C5—C6—C7	121.3 (6)	C17—C22—C23	118.4 (6)
C1—C6—C7	118.9 (7)	C32—C23—C24	118.1 (6)
C8—C7—C16	117.6 (6)	C32—C23—C22	122.3 (6)
C8—C7—C6	120.9 (6)	C24—C23—C22	119.5 (6)
C16—C7—C6	121.4 (7)	C23—C24—C25	120.7 (6)
C7—C8—C9	123.7 (7)	C23—C24—H24	119.7
C7—C8—H8	118.1	C25—C24—H24	119.7
C9—C8—H8	118.1	C30—C25—C24	120.8 (7)
C14—C9—C10	119.0 (7)	C30—C25—C26	118.7 (6)
C14—C9—C8	118.1 (7)	C24—C25—C26	120.6 (6)
C10—C9—C8	122.9 (7)	C27—C26—C25	119.0 (7)
C11—C10—C9	120.5 (7)	C27—C26—H26	120.5
C11—C10—H10	119.8	C25—C26—H26	120.5
C9—C10—H10	119.8	C28—C27—C26	122.1 (8)
C10—C11—C12	121.5 (8)	C28—C27—H27	119.0
C10—C11—H11	119.2	C26—C27—H27	119.0
C12—C11—H11	119.2	C27—C28—C29	120.2 (7)
C13—C12—C11	120.9 (8)	C27—C28—H28	119.9
C13—C12—H12	119.6	C29—C28—H28	119.9
C11—C12—H12	119.6	C28—C29—C30	120.1 (7)
C12—C13—C14	119.0 (7)	C28—C29—H29	119.9
C12—C13—H13	120.5	C30—C29—H29	119.9
C14—C13—H13	120.5	C25—C30—C29	119.9 (7)
C9—C14—C13	119.1 (7)	C25—C30—C31	118.2 (6)
C9—C14—C15	119.3 (6)	C29—C30—C31	121.9 (6)
C13—C14—C15	121.6 (6)	C32—C31—C30	119.7 (6)
C16—C15—C14	118.8 (6)	C32—C31—C15	120.0 (6)
C16—C15—C31	121.2 (6)	C30—C31—C15	120.2 (6)
C14—C15—C31	119.9 (6)	C31—C32—O2	121.9 (6)
O1—C16—C15	120.2 (6)	C31—C32—C23	122.5 (7)
O1—C16—C7	117.3 (6)	O2—C32—C23	115.6 (5)
C6—C1—C2—C3	0.2 (14)	F4—C18—C19—C20	−179.5 (8)
C6—C1—C2—F1	−179.9 (8)	C17—C18—C19—C20	1.0 (16)
C1—C2—C3—C4	0.2 (16)	F4—C18—C19—F5	−0.6 (15)
F1—C2—C3—C4	−179.7 (8)	C17—C18—C19—F5	179.9 (7)
C1—C2—C3—F2	−179.5 (8)	C18—C19—C20—F6	177.8 (10)
F1—C2—C3—F2	0.6 (15)	F5—C19—C20—F6	−1.2 (15)
F2—C3—C4—F3	1.8 (14)	C18—C19—C20—C21	−2.6 (16)
C2—C3—C4—F3	−177.9 (9)	F5—C19—C20—C21	178.4 (9)

F2—C3—C4—C5	178.9 (8)	C19—C20—C21—C22	1.7 (15)
C2—C3—C4—C5	−0.8 (15)	F6—C20—C21—C22	−178.7 (10)
C3—C4—C5—C6	0.9 (13)	C20—C21—C22—C17	0.8 (15)
F3—C4—C5—C6	178.0 (8)	C20—C21—C22—C23	179.4 (7)
C4—C5—C6—C1	−0.5 (12)	C18—C17—C22—C21	−2.3 (13)
C4—C5—C6—C7	178.1 (7)	C18—C17—C22—C23	179.0 (7)
C2—C1—C6—C5	0.0 (12)	C21—C22—C23—C32	57.0 (12)
C2—C1—C6—C7	−178.7 (7)	C17—C22—C23—C32	−124.4 (8)
C5—C6—C7—C8	−138.5 (8)	C21—C22—C23—C24	−127.2 (9)
C1—C6—C7—C8	40.1 (11)	C17—C22—C23—C24	51.5 (10)
C5—C6—C7—C16	43.8 (11)	C32—C23—C24—C25	0.1 (9)
C1—C6—C7—C16	−137.5 (7)	C22—C23—C24—C25	−175.9 (6)
C16—C7—C8—C9	2.7 (11)	C23—C24—C25—C30	−0.1 (10)
C6—C7—C8—C9	−175.0 (6)	C23—C24—C25—C26	−179.4 (6)
C7—C8—C9—C14	−3.1 (10)	C30—C25—C26—C27	0.0 (10)
C7—C8—C9—C10	177.0 (7)	C24—C25—C26—C27	179.3 (7)
C14—C9—C10—C11	0.2 (11)	C25—C26—C27—C28	−2.3 (12)
C8—C9—C10—C11	−179.9 (7)	C26—C27—C28—C29	3.2 (13)
C9—C10—C11—C12	−1.1 (12)	C27—C28—C29—C30	−1.7 (11)
C10—C11—C12—C13	0.2 (13)	C24—C25—C30—C29	−178.0 (6)
C11—C12—C13—C14	1.4 (12)	C26—C25—C30—C29	1.3 (10)
C10—C9—C14—C13	1.4 (10)	C24—C25—C30—C31	0.6 (9)
C8—C9—C14—C13	−178.4 (7)	C26—C25—C30—C31	180.0 (6)
C10—C9—C14—C15	−178.5 (6)	C28—C29—C30—C25	−0.5 (10)
C8—C9—C14—C15	1.6 (9)	C28—C29—C30—C31	−179.1 (6)
C12—C13—C14—C9	−2.2 (11)	C25—C30—C31—C32	−1.2 (9)
C12—C13—C14—C15	177.7 (6)	C29—C30—C31—C32	177.4 (6)
C9—C14—C15—C16	0.1 (9)	C25—C30—C31—C15	174.7 (6)
C13—C14—C15—C16	−179.9 (7)	C29—C30—C31—C15	−6.7 (9)
C9—C14—C15—C31	176.9 (6)	C16—C15—C31—C32	−77.4 (8)
C13—C14—C15—C31	−3.0 (10)	C14—C15—C31—C32	105.8 (8)
C14—C15—C16—O1	176.4 (6)	C16—C15—C31—C30	106.6 (8)
C31—C15—C16—O1	−0.5 (9)	C14—C15—C31—C30	−70.1 (8)
C14—C15—C16—C7	−0.5 (9)	C30—C31—C32—O2	179.5 (6)
C31—C15—C16—C7	−177.3 (7)	C15—C31—C32—O2	3.5 (10)
C8—C7—C16—O1	−177.8 (6)	C30—C31—C32—C23	1.3 (10)
C6—C7—C16—O1	0.0 (10)	C15—C31—C32—C23	−174.6 (7)
C8—C7—C16—C15	−0.8 (10)	C24—C23—C32—C31	−0.7 (10)
C6—C7—C16—C15	176.9 (6)	C22—C23—C32—C31	175.2 (6)
C22—C17—C18—C19	1.5 (14)	C24—C23—C32—O2	−179.0 (6)
C22—C17—C18—F4	−178.0 (7)	C22—C23—C32—O2	−3.1 (10)

Fig. 1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