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# 1,3-Diphenylisobenzofuran

Department of Chemistry and Biochemistry

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## Structure Reports

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## 1,3-Diphenylisobenzofuran

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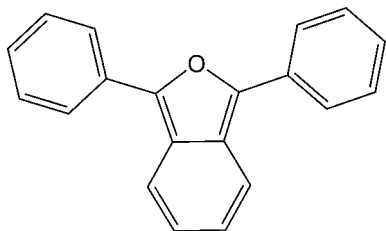
Received 26 February 2008; accepted 4 March 2008

Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.047;  $wR$  factor = 0.105; data-to-parameter ratio = 14.9.

The structure of the title compound, 1,3-diphenyl-2-benzofuran,  $\text{C}_{20}\text{H}_{14}\text{O}$ , exhibits a distinct alternation of short [mean 1.361 (3) Å] and long [mean 1.431 (3) Å] C—C bonds around the benzofuran ring system, indicating a predominantly polyene character. Over 60 Diels–Alder adducts of this commercially available furan have been structurally characterized, but this is the first report of the structure of the parent compound.

## Related literature

For related literature, see: Wege (1998); Friedrichsen (1980); Friedrichsen (1999); Allen (2002); Yang & Duan (1991); Rodrigo *et al.* (1986); Lynch *et al.* (1995); Lu *et al.* (2006).



## Experimental

## Crystal data

$\text{C}_{20}\text{H}_{14}\text{O}$   
 $M_r = 270.31$   
 Monoclinic,  $P2_1/c$   
 $a = 12.8198$  (17) Å  
 $b = 5.5273$  (8) Å  
 $c = 19.945$  (3) Å  
 $\beta = 106.480$  (2)°

$V = 1355.2$  (3) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 173$  (2) K  
 $0.28 \times 0.13 \times 0.04$  mm

## Data collection

Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2004)  
 $T_{\min} = 0.977$ ,  $T_{\max} = 0.998$

13976 measured reflections  
 2854 independent reflections  
 1664 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.085$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.105$   
 $S = 1.03$   
 2854 reflections

191 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.21$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

O1—C1	1.366 (2)	C3—C4	1.351 (3)
O1—C8	1.369 (2)	C4—C5	1.435 (3)
C1—C2	1.373 (3)	C5—C6	1.346 (3)
C2—C3	1.425 (3)	C6—C7	1.427 (3)
C2—C7	1.435 (3)	C7—C8	1.372 (3)

Data collection: APEX2 (Bruker, 2006); cell refinement: APEX2; data reduction: SAINT (Bruker, 2006); program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: publCIF (Westrip, 2008).

The Natural Sciences and Engineering Research Council of Canada is acknowledged for Discovery Grants (RTB & PWD). The diffractometer was purchased with the help of NSERC and the University of Lethbridge. The advice of C. A. Campana of Bruker AXS is also gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2071).

## References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.  
 Bruker (2006). APEX2 and SAINT. Bruker AXS, Inc., Madison, Wisconsin, USA.  
 Friedrichsen, W. (1980). *Adv. Heterocycl. Chem.* **26**, 135–241.  
 Friedrichsen, W. (1999). *Recent Advances in the Chemistry of Benzo[c]furans and Related Compounds*, Vol. 73, *Advances in Heterocyclic Chemistry*, edited by A. R. Katritzky, pp. 1–96. London: Academic Press.  
 Lu, J., Ho, D. M., Vogelaar, N. J., Kraml, C. M., Bernhard, S., Byrne, N., Kim, L. R. & Pascal, R. A. Jr (2006). *J. Am. Chem. Soc.* **128**, 17043–17050.  
 Lynch, V. M., Fairhurst, R. A., Magnus, P. & Davis, B. E. (1995). *Acta Cryst.* **C51**, 780–782.  
 Rodrigo, R., Knabe, S. M., Taylor, N. J., Rajapaksa, D. & Chernishenko, M. (1986). *J. Org. Chem.* **51**, 3973–3978.  
 Sheldrick, G. M. (2004). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Wege, D. (1998). *Aspects of the Chemistry of Isobenzofurans*, Vol. 4, *Advances in Theoretically Interesting Molecules*, edited by R. P. Thummel, pp. 1–52. Greenwich, Connecticut: J. A. I. Press.  
 Westrip, S. J. (2008). publCIF. In preparation.  
 Yang, P.-P. & Duan, W.-G. (1991). *Youji Huaxue*, **11**, 620–623.

## supporting information

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## 1,3-Diphenylisobenzofuran

René T. Boéré, Peter W. Dibble and Kristapher E. Fischer

### S1. Comment

Isobenzofuran is a ten  $\pi$ -electron system exhibiting very high reactivity in Diels-Alder reactions (Wege, 1998; Friedrichsen, 1999). The commercially available 1,3-diphenyl-2-benzofuran, (I), is a molecule with many interesting features (Friedrichsen, 1980) and unlike the parent compound is stable in the solid state. It is brightly fluorescent, electroluminescent and, despite its stability relative to isobenzofuran is still highly reactive in Diels-Alder reactions. Its reactivity is exploited in the quantitative kinetic investigations of biological singlet oxygen generation and in the *in situ* trapping of transient olefin intermediates. With respect to this latter application, the high reactivity of (I) and the crystallinity of its adducts account for the sixty-eight X-ray structures of diphenylisobenzofuran adducts that appear in the Cambridge Crystallographic Database (Allen, 2002). Surprisingly, an X-ray structure of (I) has not appeared in the literature.

Calculations have suggested that isobenzofuran has a low resonance energy (Yang & Duan, 1991) and mainly polyene character. The structures of isobenzofurans are of interest since the degree of bond length alternation serves to indicate the balance between aromatic and polyene character. Only three structures of isobenzofurans have been published previously: 1-cyano-4,5-methylenedioxyisobenzofuran (Rodrigo *et al.*, 1986); 3,6-dimethoxyisobenzofuran (Lynch *et al.*, 1995) and the highly strained 9,10,12,13-tetraphenyl-11-oxacyclopenta[*b*]triphenylene (Lu *et al.*, 2006). All three structures show that the isobenzofuran core is essentially polyene in character with the structure of the furan ring very similar to that of furan itself.

The structure of (I) (Fig. 1) is very closely comparable to those of the three previously published examples. There is no significant evidence of bond length averaging indicating that it has predominantly polyene character. Of the three published structures, the bond lengths of (I) are closest to those calculated for the parent compound using the MP2/6–31G\* basis set (Friedrichsen, 1980). The only noticeable difference is in the C1—C2, C7—C8 bonds which are slightly longer, perhaps the effect of conjugation to the phenyl substituents. While the most recent structure (Lu *et al.*, 2006) contains the diphenylisobenzofuran substructure, extensive *peri* interactions throughout the molecule lead to significant deviations from planarity making direct structural comparisons less meaningful.

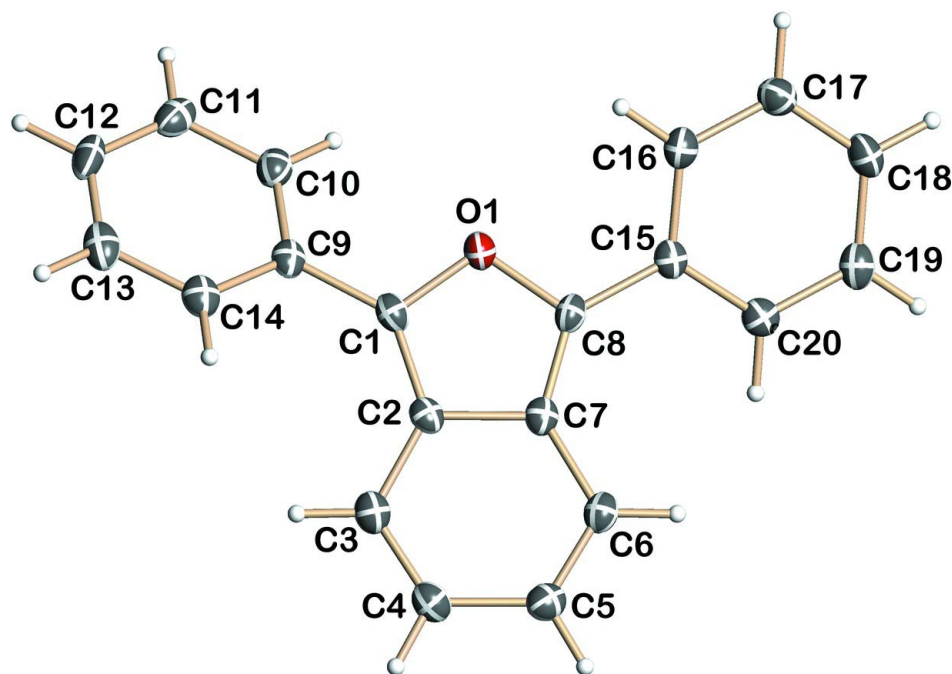
Strong steric interactions between the phenyl substituents of (I) and the *peri* H atoms (H3 and H6) are indicated by a 25° torsional twist of the phenyl rings out of the plane of the isobenzofuran ring and wide 135.3 (2)° and 135.5 (2)° bond angles for C2—C1—C9, C7—C8—C15.

### S2. Experimental

Commercial 1,3-diphenyl-2-benzofuran [CAS-5471-66-6] (Aldrich) was recrystallized from ethanol.

### S3. Refinement

The space group was determined by trial and error and confirmed by a successful refinement. The alternative choice,  $Pc$ , gave unrealistic geometrical parameters. H-atoms were included at geometrically idealized positions with C—H distance 0.95 Å and  $U_{\text{iso}} = 1.2$  times  $U_{\text{eq}}$  of the C-atoms to which they were bonded. The model was refined to convergence, and there were no chemically significant features on the final difference Fourier map.



**Figure 1**

Thermal ellipsoid plot of the structure of (I) drawn at 50% probability level showing the atom numbering scheme.

### 1,3-diphenyl-2-benzofuran

#### Crystal data

$C_{20}H_{14}O$   
 $M_r = 270.31$   
 Monoclinic,  $P2_1/c$   
 Hall symbol:  $-P 2_1/c$   
 $a = 12.8198$  (17) Å  
 $b = 5.5273$  (8) Å  
 $c = 19.945$  (3) Å  
 $\beta = 106.480$  (2)°  
 $V = 1355.2$  (3) Å<sup>3</sup>  
 $Z = 4$

$F(000) = 568$   
 $D_x = 1.325$  Mg m<sup>-3</sup>  
 Melting point: 128 K  
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å  
 Cell parameters from 2945 reflections  
 $\theta = 2.3$ – $24.1$ °  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 173$  K  
 Plate, green  
 $0.28 \times 0.13 \times 0.04$  mm

#### Data collection

Bruker APEXII CCD area-detector  
 diffractometer  
 Radiation source: fine-focus sealed tube, fixed  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
 (*SADABS*; Sheldrick, 2004)  
 $T_{\text{min}} = 0.977$ ,  $T_{\text{max}} = 0.998$   
 13976 measured reflections  
 2854 independent reflections  
 1664 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.085$   
 $\theta_{\text{max}} = 26.7^\circ$ ,  $\theta_{\text{min}} = 2.1^\circ$   
 $h = -16 \rightarrow 16$

$k = -6 \rightarrow 6$   
 $l = -25 \rightarrow 25$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.105$   
 $S = 1.03$   
 2854 reflections  
 191 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods  
 Secondary atom site location: difference Fourier  
 map

Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0358P)^2 + 0.3395P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.20 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.21 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: *SHELXTL* (Sheldrick,  
 2008),  $F_c^* = kFc[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0103 (12)

*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. 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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.29644 (11)	0.9505 (2)	0.35614 (7)	0.0205 (4)
C1	0.21954 (16)	0.8022 (4)	0.31456 (11)	0.0202 (5)
C2	0.20930 (16)	0.8560 (4)	0.24577 (11)	0.0196 (5)
C3	0.14208 (17)	0.7650 (4)	0.18104 (11)	0.0218 (5)
H3	0.0905	0.6406	0.1801	0.026*
C4	0.15333 (17)	0.8597 (4)	0.12105 (12)	0.0240 (5)
H4	0.1089	0.8002	0.0776	0.029*
C5	0.23051 (17)	1.0476 (4)	0.12106 (11)	0.0245 (5)
H5	0.2363	1.1087	0.0777	0.029*
C6	0.29489 (17)	1.1392 (4)	0.18114 (11)	0.0234 (5)
H6	0.3461	1.2628	0.1804	0.028*
C7	0.28490 (16)	1.0474 (4)	0.24591 (11)	0.0191 (5)
C8	0.33653 (16)	1.0998 (4)	0.31456 (11)	0.0203 (5)
C9	0.16786 (16)	0.6343 (4)	0.35090 (11)	0.0187 (5)
C10	0.16433 (16)	0.6805 (4)	0.41877 (11)	0.0236 (5)
H10	0.1966	0.8240	0.4418	0.028*
C11	0.11450 (17)	0.5203 (4)	0.45328 (12)	0.0256 (5)

H11	0.1140	0.5527	0.5000	0.031*
C12	0.06547 (17)	0.3130 (4)	0.41987 (11)	0.0265 (6)
H12	0.0300	0.2046	0.4432	0.032*
C13	0.06827 (17)	0.2643 (4)	0.35262 (12)	0.0246 (5)
H13	0.0349	0.1216	0.3297	0.030*
C14	0.11927 (16)	0.4218 (4)	0.31841 (11)	0.0214 (5)
H14	0.1214	0.3856	0.2723	0.026*
C15	0.42170 (17)	1.2651 (4)	0.35097 (11)	0.0204 (5)
C16	0.48555 (17)	1.2125 (4)	0.41833 (11)	0.0241 (5)
H16	0.4722	1.0692	0.4409	0.029*
C17	0.56847 (17)	1.3671 (4)	0.45278 (12)	0.0273 (6)
H17	0.6113	1.3302	0.4989	0.033*
C18	0.58898 (18)	1.5752 (4)	0.42018 (12)	0.0285 (6)
H18	0.6464	1.6803	0.4436	0.034*
C19	0.52636 (17)	1.6294 (4)	0.35396 (12)	0.0281 (6)
H19	0.5407	1.7721	0.3316	0.034*
C20	0.44235 (17)	1.4777 (4)	0.31940 (12)	0.0243 (5)
H20	0.3985	1.5189	0.2739	0.029*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0184 (8)	0.0201 (8)	0.0231 (8)	-0.0025 (6)	0.0062 (7)	0.0010 (7)
C1	0.0161 (11)	0.0185 (12)	0.0258 (13)	-0.0009 (9)	0.0058 (10)	-0.0030 (10)
C2	0.0163 (11)	0.0172 (11)	0.0257 (13)	0.0014 (9)	0.0065 (10)	-0.0009 (9)
C3	0.0190 (12)	0.0185 (11)	0.0272 (13)	0.0002 (9)	0.0055 (10)	-0.0018 (10)
C4	0.0213 (12)	0.0256 (13)	0.0248 (13)	0.0016 (10)	0.0059 (10)	-0.0023 (10)
C5	0.0231 (12)	0.0249 (12)	0.0266 (13)	0.0033 (10)	0.0090 (10)	0.0046 (10)
C6	0.0207 (12)	0.0219 (12)	0.0281 (13)	0.0003 (10)	0.0076 (10)	0.0023 (10)
C7	0.0185 (11)	0.0179 (11)	0.0228 (12)	0.0027 (9)	0.0089 (10)	0.0002 (9)
C8	0.0209 (12)	0.0173 (12)	0.0252 (13)	0.0020 (9)	0.0105 (10)	0.0040 (9)
C9	0.0145 (10)	0.0178 (11)	0.0233 (12)	0.0027 (9)	0.0046 (9)	0.0032 (9)
C10	0.0203 (12)	0.0226 (12)	0.0265 (13)	-0.0024 (9)	0.0045 (10)	-0.0001 (10)
C11	0.0258 (12)	0.0276 (13)	0.0235 (12)	-0.0004 (10)	0.0071 (10)	0.0019 (10)
C12	0.0254 (13)	0.0249 (13)	0.0308 (14)	-0.0011 (10)	0.0107 (11)	0.0064 (11)
C13	0.0196 (12)	0.0196 (12)	0.0342 (14)	0.0005 (10)	0.0067 (11)	0.0020 (10)
C14	0.0183 (11)	0.0211 (12)	0.0239 (12)	0.0038 (9)	0.0045 (10)	0.0019 (10)
C15	0.0168 (11)	0.0196 (12)	0.0265 (13)	0.0014 (9)	0.0092 (10)	-0.0031 (10)
C16	0.0228 (12)	0.0232 (13)	0.0271 (13)	-0.0021 (10)	0.0084 (10)	-0.0038 (10)
C17	0.0203 (12)	0.0334 (14)	0.0277 (13)	0.0002 (10)	0.0060 (10)	-0.0088 (11)
C18	0.0216 (12)	0.0260 (14)	0.0397 (15)	-0.0069 (10)	0.0119 (11)	-0.0146 (11)
C19	0.0275 (13)	0.0188 (13)	0.0428 (16)	-0.0005 (10)	0.0178 (12)	-0.0031 (11)
C20	0.0228 (12)	0.0211 (12)	0.0313 (13)	0.0025 (10)	0.0113 (10)	-0.0001 (10)

*Geometric parameters (Å, °)*

O1—C1	1.366 (2)	C10—H10	0.9500
O1—C8	1.369 (2)	C11—C12	1.384 (3)

C1—C2	1.373 (3)	C11—H11	0.9500
C1—C9	1.449 (3)	C12—C13	1.379 (3)
C2—C3	1.425 (3)	C12—H12	0.9500
C2—C7	1.435 (3)	C13—C14	1.380 (3)
C3—C4	1.351 (3)	C13—H13	0.9500
C3—H3	0.9500	C14—H14	0.9500
C4—C5	1.435 (3)	C15—C16	1.391 (3)
C4—H4	0.9500	C15—C20	1.394 (3)
C5—C6	1.346 (3)	C16—C17	1.385 (3)
C5—H5	0.9500	C16—H16	0.9500
C6—C7	1.427 (3)	C17—C18	1.383 (3)
C6—H6	0.9500	C17—H17	0.9500
C7—C8	1.372 (3)	C18—C19	1.370 (3)
C8—C15	1.451 (3)	C18—H18	0.9500
C9—C10	1.391 (3)	C19—C20	1.384 (3)
C9—C14	1.399 (3)	C19—H19	0.9500
C10—C11	1.384 (3)	C20—H20	0.9500
C1—O1—C8	108.91 (16)	C12—C11—C10	120.1 (2)
O1—C1—C2	108.95 (18)	C12—C11—H11	120.0
O1—C1—C9	115.74 (18)	C10—C11—H11	120.0
C2—C1—C9	135.3 (2)	C13—C12—C11	119.8 (2)
C1—C2—C3	133.7 (2)	C13—C12—H12	120.1
C1—C2—C7	106.53 (18)	C11—C12—H12	120.1
C3—C2—C7	119.77 (19)	C12—C13—C14	120.3 (2)
C4—C3—C2	118.5 (2)	C12—C13—H13	119.8
C4—C3—H3	120.8	C14—C13—H13	119.8
C2—C3—H3	120.8	C13—C14—C9	120.8 (2)
C3—C4—C5	121.8 (2)	C13—C14—H14	119.6
C3—C4—H4	119.1	C9—C14—H14	119.6
C5—C4—H4	119.1	C16—C15—C20	118.5 (2)
C6—C5—C4	121.4 (2)	C16—C15—C8	120.30 (19)
C6—C5—H5	119.3	C20—C15—C8	121.2 (2)
C4—C5—H5	119.3	C17—C16—C15	120.6 (2)
C5—C6—C7	118.8 (2)	C17—C16—H16	119.7
C5—C6—H6	120.6	C15—C16—H16	119.7
C7—C6—H6	120.6	C18—C17—C16	120.1 (2)
C8—C7—C6	133.4 (2)	C18—C17—H17	119.9
C8—C7—C2	106.96 (18)	C16—C17—H17	119.9
C6—C7—C2	119.64 (19)	C19—C18—C17	119.8 (2)
O1—C8—C7	108.65 (18)	C19—C18—H18	120.1
O1—C8—C15	115.80 (18)	C17—C18—H18	120.1
C7—C8—C15	135.5 (2)	C18—C19—C20	120.5 (2)
C10—C9—C14	118.14 (19)	C18—C19—H19	119.7
C10—C9—C1	121.01 (19)	C20—C19—H19	119.7
C14—C9—C1	120.86 (19)	C19—C20—C15	120.4 (2)
C11—C10—C9	120.9 (2)	C19—C20—H20	119.8
C11—C10—H10	119.5	C15—C20—H20	119.8

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C9—C10—H10	119.5		
C8—O1—C1—C2	-0.2 (2)	C2—C1—C9—C10	-155.0 (2)
C8—O1—C1—C9	-179.21 (16)	O1—C1—C9—C14	-156.91 (17)
O1—C1—C2—C3	-178.8 (2)	C2—C1—C9—C14	24.5 (4)
C9—C1—C2—C3	-0.2 (4)	C14—C9—C10—C11	0.2 (3)
O1—C1—C2—C7	0.2 (2)	C1—C9—C10—C11	179.72 (19)
C9—C1—C2—C7	178.9 (2)	C9—C10—C11—C12	-1.2 (3)
C1—C2—C3—C4	-179.7 (2)	C10—C11—C12—C13	1.3 (3)
C7—C2—C3—C4	1.4 (3)	C11—C12—C13—C14	-0.3 (3)
C2—C3—C4—C5	0.0 (3)	C12—C13—C14—C9	-0.7 (3)
C3—C4—C5—C6	-0.4 (3)	C10—C9—C14—C13	0.7 (3)
C4—C5—C6—C7	-0.5 (3)	C1—C9—C14—C13	-178.76 (19)
C5—C6—C7—C8	-179.9 (2)	O1—C8—C15—C16	23.8 (3)
C5—C6—C7—C2	1.8 (3)	C7—C8—C15—C16	-154.2 (2)
C1—C2—C7—C8	-0.2 (2)	O1—C8—C15—C20	-156.92 (18)
C3—C2—C7—C8	179.07 (19)	C7—C8—C15—C20	25.1 (4)
C1—C2—C7—C6	178.52 (19)	C20—C15—C16—C17	-0.7 (3)
C3—C2—C7—C6	-2.3 (3)	C8—C15—C16—C17	178.64 (19)
C1—O1—C8—C7	0.1 (2)	C15—C16—C17—C18	-0.4 (3)
C1—O1—C8—C15	-178.40 (16)	C16—C17—C18—C19	0.7 (3)
C6—C7—C8—O1	-178.4 (2)	C17—C18—C19—C20	0.2 (3)
C2—C7—C8—O1	0.0 (2)	C18—C19—C20—C15	-1.3 (3)
C6—C7—C8—C15	-0.3 (4)	C16—C15—C20—C19	1.5 (3)
C2—C7—C8—C15	178.1 (2)	C8—C15—C20—C19	-177.77 (19)
O1—C1—C9—C10	23.6 (3)		

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