Table 2. *Selected geometric parameters (Å, °)*

C1—C2	1.358 (2)	B1—O1	1.366 (2)
C1—C41	1.496 (2)	B1—O2	1.370 (2)
C1—B1	1.580 (2)	B2—O3	1.366 (2)
C2—C31	1.496 (2)	B2—O4	1.371 (2)
C2—B2	1.564 (2)		
C2—C1—C41	124.04 (11)	O2—B1—C1	122.88 (11)
C2—C1—B1	124.15 (11)	B1—O1—C11	106.70 (10)
C41—C1—B1	111.79 (10)	B1—O2—C12	106.86 (10)
C1—C2—C31	123.82 (11)	O3—B2—O4	113.38 (11)
C1—C2—B2	119.30 (11)	O3—B2—C2	123.94 (11)
C31—C2—B2	116.87 (10)	O4—B2—C2	122.64 (11)
O1—B1—O2	113.35 (11)	B2—O3—C21	106.92 (10)
O1—B1—C1	123.03 (11)	B2—O4—C22	106.74 (10)

The data collection nominally covered more than a hemisphere of reciprocal space. Coverage of the unique set is virtually complete to at least 26.4° in θ. Crystal decay was monitored by repeating the initial frames at the end of data collection and analysing the duplicate reflections.

H atoms were placed geometrically and refined with a riding model and with $U_{\rm iso}$ constrained to be 1.2 (1.5 for methyl groups) times $U_{\rm eq}$ of the carrier atom. The combination of X-ray wavelength and elements present in the compound does not permit a reliable determination of the absolute structure (Flack, 1983).

Data collection: *SMART* (Siemens, 1995). Cell refinement: local programs. Data reduction: *SAINT* (Siemens, 1995). Program(s) used to solve structure: *SHELXTL* (Sheldrick, 1994). Program(s) used to refine structure: *SHELXTL*. Molecular graphics: *SHELXTL*. Software used to prepare material for publication: *SHELXTL* and local programs.

We thank EPSRC (UK) and NSERC (Canada) for support of this research, and NSERC, the Royal Society (UK), the British Council (Ottawa) and the University of Newcastle for Bilateral Exchange awards, travel grants and fellowships to support the collaboration.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1368). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1996). C**52**, 1991–1995

The Products of Catalysed Diboration of Bis(*p*-tolyl)ethyne and of 4-Cyanophenylethyne by Bis(catecholato-*O*,*O*′)diboron

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(*Received 17 April 1996; accepted 17 May 1996*)

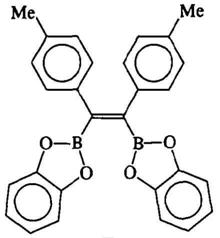
Abstract

Both (*Z*)-1,2-bis(1,3,2-benzodioxaborolan-2-yl)-1,2-bis(4-methylphenyl)ethene [(I), $C_{28}H_{22}B_2O_4$] and (*Z*)-4-[1,2-bis(1,3,2-benzodioxaborolan-2-yl)vinyl]benzonitrile [(II), $C_{21}H_{13}B_2NO_4$] have a *cis* arrangement of two boronate ester substituents on a C═C double bond, which shows a slight twist to relieve steric crowding of the substituents. The interplay of steric and electronic factors results in approximate coplanarity of only one substituent with the alkene unit in (I), while this is achieved for two mutually *trans* substituents in the less crowded (II). A consistent pattern of bonding and conformational geometry is found for a series of related alkenes with boronate ester substituents. The catecholboronate group shows almost invariant geometry across a range of compounds, with a slight but probably real lengthening of the B—O bonds on coordination to transition metals.

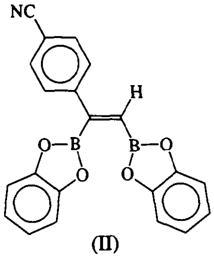
Comment

The addition of B—B bonds to alkynes is catalyzed by platinum bis(phosphine) complexes and leads to *cis*-alkene-1,2-bis(boronate esters) (Ishiyama, Matsuda, Miyaura & Suzuki, 1993; Iverson & Smith, 1995; Lesley *et al.*, 1996; Ishiyama *et al.*, 1996). We have reported previously the structure of one product of addition of bis(pinacolato-*O*,*O*′)diboron, B_2pin_2, to a symmetrical alkyne (Clegg, Scott, Lesley, Marder & Norman, 1996) and of representative products of addition of bis(catecholato-*O*,*O*′)diboron, B_2cat_2, to an internal alkyne, a terminal alkyne, and a 1,3-diyne (Lesley *et al.*, 1996). We report here the structures of two further adducts of B_2cat_2 with alkynes, with an analysis of the whole series of related structures and other molecules containing the Bcat unit, including the starting material B_2cat_2 itself (Nguyen *et al.*, 1994).

Acta Crystallographica Section C
ISSN 0108-2701 © 1996



(I)



(II)

Both molecules have an essentially planar central B_2C_3H or B_2C_4 unit with a *cis* disposition of the boronate ester groups at the alkene C=C bond. For (II) the r.m.s. deviation of the C and B atoms in this unit is 0.028 (2) Å, with a B1—C1—C2—B2 torsion angle of −7.9 (1)°, representing a slight twist; for (I) the corresponding r.m.s. deviation is 0.026 (2) Å, and the B1—C1—C2—B2 and C31—C1—C2—C41 torsion angles are 0.5 (1) and 5.6 (1)°, respectively. Similar minor twisting deformations about the C=C double bond were found for the related compounds (III) [which has a *p*-OMe group in place of the *p*-CN group of (II)], (IV) [which has two unsubstituted phenyl groups in place of the *p*-tolyl groups of (I)], and (V) (which is a 1,3-diene with two *cis*-Bcat groups and one terminal *p*-methoxyphenyl group on each double bond) (Lesley *et al.*, 1996), as well as for the adduct of B_2pin_2 with bis(4-methoxyphenyl)ethyne, (VI) (Clegg *et al.*, 1996).

In both the terminal alkene compounds (II) and (III), the central alkene unit is approximately coplanar with its carbon substituent and with the boronate group attached to C—H, while the other boronate group is rotated roughly perpendicular to this plane [in (II) the dihedral angles for these substituents relative to the alkene mean plane are 16.8 (2), 8.6 (2) and 80.4 (2)°, respectively]. In both the internal alkene compounds (I) and (IV), approximate coplanarity with the alkene unit is achieved only by one boronate group [in (I) the relevant dihedral angles are 16.3 (2)° for the B2 boronate group, 75.4 (2)° for the B1 boronate group, and 52.7 (2) and 46.4 (2)° for the C31 and C41 aryl groups, respectively]. In the diene (V), the two terminal boronate groups are approximately coplanar with their respective alkene units, while the other two boronate groups and all four aryl groups are roughly perpendicular to them. This consistent pattern for the series as a whole is a consequence of the compromise between steric interaction of the various alkene substituent groups and the stabilizing effect of bringing substituents into coplanarity and hence effective conjugation with the alkene.

Consistent effects of these steric and electronic factors can also be seen in some of the bond lengths and angles of the five compounds. The C=C bond lengths are shortest for the terminal alkenes [1.349 (2) for (II), 1.348 (2) Å for (III)], intermediate for the symmetrical internal alkenes [1.357 (2) for (I), 1.353 (2) and 1.358 (2) Å for the two independent molecules of (IV)], and longest for the diene [1.373 (3) and 1.362 (2) Å for the two double bonds of (V)]. The value for (VI), another symmetrical internal alkene, is 1.358 (2) Å. Steric crowding is relieved in the terminal alkenes by an opening up of the B—C=C angle at the unsubstituted C atom relative to that at the substituted C atom.

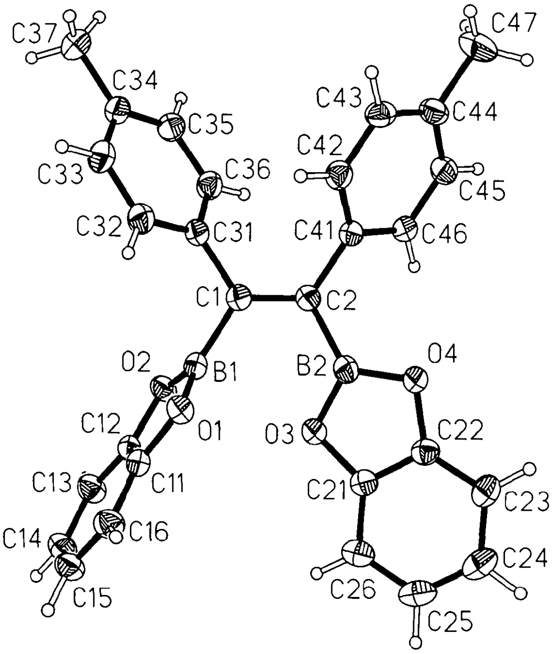


Fig. 1. The molecular structure of (I) with atom labels and 50% probability ellipsoids for non-H atoms.

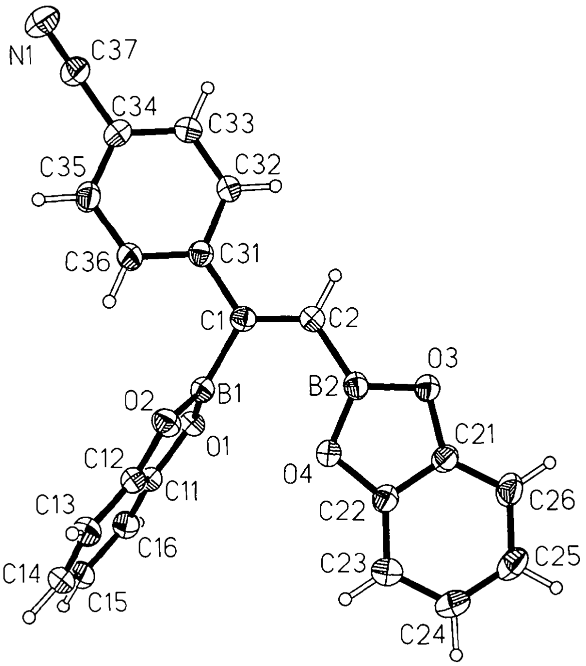


Fig. 2. The molecular structure of (II) with atom labels and 50% probability ellipsoids for non-H atoms.

The internal geometry of the Bcat groups remains remarkably constant across the whole series, not only of these five structures, but also of 15 others in the Cambridge Structural Database (Allen & Kennard, 1993) and four others reported by Lesley *et al.* (1996) and Dai *et al.* (1996), which have Bcat bonded to one other atom; the 24 structures contain a total of 44 Bcat groups. The r.m.s. deviation of the atoms of the BO_2C_2 ring from their mean plane does not exceed 0.025 Å in any of the groups, with O—C—C—O torsion angles always <3°. B—O bonds lie within the narrow range 1.376–1.407 Å when boron is bonded to a non-metal (B, C, N or O) [for the five alkene compounds, the B—O range is particularly narrow, with a minimum of 1.3798 (14) Å in (II) and a maximum of 1.393 (2) Å in both (IV) and (V)], and within the range 1.387–1.444 Å (with rather higher estimated standard deviations in general) when boron is bonded to a transition metal (Fe, Rh, Ta, W, Ir or Pt); the lengthening in the metal complexes is only slight but probably real, since the overall distribution is clearly bimodal. In all the compounds, O—C bond lengths and angles at both boron and oxygen are very similar to those reported here for (I) and (II).

Experimental

Compounds (I) and (II) were prepared by platinum-catalysed addition of bis(catecholato-*O*,*O*′)diboron (B_2cat_2) to bis(*p*-tolyl)ethyne and to 4-cyanophenylethyne, respectively, with the general method described by Lesley *et al.* (1996). For (I), bis(*p*-tolyl)ethyne (400 mg, 1.9 mmol), B_2cat_2 (462 mg, 1.9 mmol) and $[(PPh_3)_2Pt(Bcat)_2].C_7H_8$ (80 mg, 7.6 × 10^{-5} mol) were heated to 363 K in toluene (15 cm^3) under nitrogen gas for 2 days; the solid product was collected by filtration, and washed with hexanes. For (II), 4-cyanophenylethyne (50 mg, 0.4 mmol), B_2cat_2 (94 mg, 0.4 mmol) and $[(PPh_3)_2Pt(\eta\text{-}C_2H_4)]$ (30 mg, 4.0 × 10^{-5} mol) were heated to 373 K in toluene (5 cm^3) for 2 h; the solid product was collected by filtration. Crystals of each product were produced by diffusion of a layer of hexanes into a solution in toluene. Appropriate ^1H and ^{13}C NMR spectroscopic results were obtained.

Compound (I)

Crystal data

$C_{28}H_{22}B_2O_4$
$M_r = 444.08$
Monoclinic
$P2_1/c$
$a = 9.5156 (9)$ Å
$b = 22.206 (2)$ Å
$c = 11.6192 (10)$ Å
$\beta = 108.059 (2)°$
$V = 2334.2 (4)$ Å^3
$Z = 4$
$D_x = 1.264$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 9049 reflections
$\theta = 2.06–28.17°$
$\mu = 0.082$ mm^{-1}
$T = 160 (2)$ K
Block
0.70 × 0.56 × 0.14 mm
Colourless

Data collection

Siemens SMART CCD diffractometer
Sets of exposures each taken over 0.3° ω rotation
Absorption correction: none
14334 measured reflections
5276 independent reflections

4454 observed reflections $[I > 2\sigma(I)]$
$R_{int} = 0.0252$
$\theta_{max} = 28.39°$
$h = -11 \rightarrow 12$
$k = -29 \rightarrow 14$
$l = -14 \rightarrow 14$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0385$
$wR(F^2) = 0.0999$
$S = 1.070$
5271 reflections
310 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0370P)^2 + 0.8484P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = -0.001$
$\Delta\rho_{max} = 0.317$ e Å^{-3}
$\Delta\rho_{min} = -0.198$ e Å^{-3}

Extinction correction: *SHELXTL* (Sheldrick, 1994)
Extinction coefficient: 0.0045 (7)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for (I)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
C1	0.22560 (14)	0.36001 (5)	0.32048 (11)	0.0260 (3)
C2	0.25706 (13)	0.30184 (5)	0.30219 (11)	0.0259 (3)
B1	0.3063 (2)	0.41426 (6)	0.28226 (13)	0.0261 (3)
O1	0.27375 (10)	0.43696 (4)	0.16578 (8)	0.0286 (2)
O2	0.41179 (10)	0.44890 (4)	0.36463 (8)	0.0294 (2)
C11	0.36810 (14)	0.48567 (5)	0.17592 (11)	0.0256 (3)
C12	0.45023 (14)	0.49335 (5)	0.29573 (11)	0.0266 (3)
C13	0.5520 (2)	0.53907 (6)	0.33330 (12)	0.0341 (3)
C14	0.5689 (2)	0.57697 (6)	0.24291 (13)	0.0362 (3)
C15	0.4873 (2)	0.56878 (6)	0.12225 (13)	0.0353 (3)
C16	0.3837 (2)	0.52261 (6)	0.08565 (12)	0.0325 (3)
B2	0.3786 (2)	0.28869 (6)	0.24211 (13)	0.0265 (3)
O3	0.48055 (10)	0.33119 (4)	0.23055 (8)	0.0288 (2)
O4	0.39697 (10)	0.23435 (4)	0.19008 (8)	0.0291 (2)
C21	0.56005 (14)	0.30266 (6)	0.16444 (11)	0.0276 (3)
C22	0.50954 (14)	0.24419 (6)	0.14002 (11)	0.0278 (3)
C23	0.5645 (2)	0.20537 (7)	0.07214 (13)	0.0353 (3)
C24	0.6741 (2)	0.22859 (7)	0.02808 (13)	0.0399 (3)
C25	0.7253 (2)	0.28699 (7)	0.05290 (13)	0.0403 (3)
C26	0.66960 (15)	0.32577 (7)	0.12295 (13)	0.0352 (3)
C31	0.11719 (14)	0.37847 (5)	0.38318 (11)	0.0265 (3)
C32	0.0086 (2)	0.42132 (6)	0.33186 (13)	0.0335 (3)
C33	−0.0934 (2)	0.43808 (6)	0.38919 (14)	0.0376 (3)
C34	−0.0886 (2)	0.41379 (6)	0.50094 (13)	0.0335 (3)
C35	0.0225 (2)	0.37240 (6)	0.55374 (13)	0.0331 (3)
C36	0.12349 (15)	0.35483 (6)	0.49594 (12)	0.0305 (3)
C37	−0.1991 (2)	0.43205 (7)	0.5637 (2)	0.0451 (4)
C41	0.17790 (14)	0.24916 (5)	0.33259 (11)	0.0250 (2)
C42	0.02429 (14)	0.24794 (6)	0.30369 (12)	0.0296 (3)
C43	−0.04762 (14)	0.19854 (6)	0.33185 (12)	0.0319 (3)
C44	0.0310 (2)	0.14875 (6)	0.39091 (12)	0.0326 (3)
C45	0.1843 (2)	0.14960 (6)	0.41884 (12)	0.0316 (3)
C46	0.25646 (14)	0.19859 (6)	0.38895 (11)	0.0270 (3)
C47	−0.0470 (2)	0.09490 (8)	0.4224 (2)	0.0495 (4)

Compound (II)

Crystal data

$C_{21}H_{13}B_2NO_4$
$M_r = 364.94$

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Monoclinic
$P2_1/c$
$a = 16.2526$ (14) Å
$b = 13.0229$ (12) Å
$c = 8.5856$ (8) Å
$\beta = 104.920$ (2)°
$V = 1755.9$ (3) Å^3
$Z = 4$
$D_x = 1.380$ Mg m^{-3}
D_m not measured

Cell parameters from 7574 reflections
$\theta = 2.46$–28.40°
$\mu = 0.094$ mm^{-1}
$T = 160$ (2) K
Block
0.65 × 0.60 × 0.26 mm
Yellow

Data collection

Siemens SMART CCD diffractometer
Sets of exposures each taken over 0.3° ω rotation
Absorption correction: none
10438 measured reflections
3984 independent reflections

3477 observed reflections $[I > 2\sigma(I)]$
$R_{\rm int} = 0.0244$
$\theta_{\rm max} = 28.45°$
$h = -16 \rightarrow 20$
$k = -17 \rightarrow 12$
$l = -11 \rightarrow 11$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0354$
$wR(F^2) = 0.0963$
$S = 1.031$
3980 reflections
254 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 0.5485P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.251$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.203$ e Å^{-3}

Extinction correction: *SHELXTL* (Sheldrick, 1994)
Extinction coefficient: 0.0127 (11)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 2. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (II)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
C1	0.25316 (7)	0.18996 (8)	0.29979 (13)	0.0244 (2)
C2	0.19520 (7)	0.20460 (9)	0.15777 (13)	0.0267 (2)
B1	0.26556 (8)	0.08106 (9)	0.38065 (14)	0.0256 (2)
O1	0.21156 (5)	0.04321 (6)	0.46857 (9)	0.0273 (2)
O2	0.33327 (5)	0.01586 (6)	0.38699 (10)	0.0307 (2)
C11	0.24731 (7)	−0.04965 (8)	0.53091 (13)	0.0281 (2)
C12	0.32092 (7)	−0.06575 (8)	0.48265 (13)	0.0295 (2)
C13	0.37196 (9)	−0.15025 (10)	0.5311 (2)	0.0385 (3)
C14	0.34418 (9)	−0.21912 (10)	0.6321 (2)	0.0439 (3)
C15	0.27057 (9)	−0.20244 (10)	0.6810 (2)	0.0435 (3)
C16	0.21934 (8)	−0.11618 (10)	0.6304 (2)	0.0369 (3)
B2	0.14631 (8)	0.11632 (10)	0.05614 (15)	0.0268 (3)
O3	0.08737 (5)	0.12779 (6)	−0.09176 (10)	0.0309 (2)
O4	0.15934 (5)	0.01314 (6)	0.09762 (9)	0.0307 (2)
C21	0.06359 (7)	0.02877 (9)	−0.14295 (14)	0.0285 (2)
C22	0.10696 (7)	−0.04028 (9)	−0.02898 (13)	0.0282 (2)
C23	0.09523 (9)	−0.14456 (10)	−0.0472 (2)	0.0382 (3)
C24	0.03698 (8)	−0.17746 (10)	−0.1877 (2)	0.0394 (3)
C25	−0.00681 (8)	−0.10871 (11)	−0.3015 (2)	0.0396 (3)
C26	0.00547 (8)	−0.00287 (10)	−0.2813 (2)	0.0382 (3)
C31	0.30642 (7)	0.27385 (8)	0.39171 (12)	0.0243 (2)
C32	0.28718 (7)	0.37802 (8)	0.35879 (13)	0.0274 (2)
C33	0.33628 (7)	0.45450 (9)	0.44938 (14)	0.0304 (2)
C34	0.40613 (7)	0.42822 (9)	0.57564 (14)	0.0288 (2)
C35	0.42668 (7)	0.32547 (9)	0.60940 (14)	0.0315 (3)
C36	0.37717 (7)	0.24955 (9)	0.51805 (13)	0.0291 (2)
C37	0.45698 (7)	0.50826 (10)	0.6707 (2)	0.0335 (3)
N1	0.49664 (7)	0.57274 (9)	0.7442 (2)	0.0445 (3)

Table 3. *Selected geometric parameters (Å, °) for (I) and (II)*

	(I)	(II)
C1—C2	1.357 (2)	1.349 (2)
C1—C31	1.493 (2)	1.4880 (15)
C1—B1	1.565 (2)	1.569 (2)
C2—C41	1.492 (2)	-
C2—B2	1.553 (2)	1.535 (2)
B1—O1	1.386 (2)	1.3872 (15)
B1—O2	1.386 (2)	1.3798 (14)
B2—O3	1.389 (2)	1.3879 (14)
B2—O4	1.385 (2)	1.3922 (15)
C2—C1—C31	123.85 (11)	123.45 (10)
C2—C1—B1	122.45 (11)	120.54 (10)
C31—C1—B1	113.64 (10)	115.98 (9)
C1—C2—C41	123.85 (11)	-
C1—C2—B2	118.72 (11)	123.14 (10)
C41—C2—B2	117.39 (10)	-
O1—B1—O2	111.54 (11)	111.70 (10)
O1—B1—C1	125.19 (12)	122.33 (10)
O2—B1—C1	123.06 (11)	125.73 (10)
O3—B2—O4	111.30 (11)	111.20 (10)
O3—B2—C2	123.74 (11)	125.00 (10)
O4—B2—C2	124.93 (11)	123.71 (10)
B1—O1—C11	104.95 (10)	105.00 (9)
B1—O2—C12	105.08 (10)	105.02 (9)
B2—O3—C21	105.09 (10)	105.10 (9)
B2—O4—C22	105.34 (10)	105.19 (9)

The data collection nominally covered over a hemisphere of reciprocal space in each case. Coverage of the unique set is virtually complete to at least 26.3° in θ, by a combination of three sets of exposures; each set had a different φ angle for the crystal and each exposure covered 0.3° in ω. The crystal–detector distance was 4.941 cm. Crystal decay was monitored by repeating the intial exposures at the end of data collection and analysing the duplicate reflections.

H atoms were placed geometrically and refined with a riding model and with $U_{\rm iso}$ constrained to be 1.2 (1.5 for methyl groups) times $U_{\rm eq}$ of the carrier atom.

For both compounds, data collection: *SMART* (Siemens, 1995); cell refinement: local programs; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structures: *SHELXTL* (Sheldrick, 1994); program(s) used to refine structures: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

We thank EPSRC (UK) and NSERC (Canada) for support of this research, and NSERC, the Royal Society (UK), the British Council (Ottawa) and the University of Newcastle for Bilateral Exchange awards, travel grants and fellowships to support the collaboration.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1383). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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β-Zearalenol Sesquihydrate†

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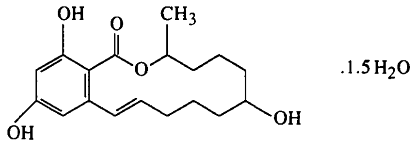
(*Received 1 April 1996; accepted 14 May 1996*)

Abstract

This X-ray diffraction study establishes the molecular structure of the title compound, 3,4,5,6,7,8,9,10-octahydro-7,14,16-trihydroxy-3-methyl-1*H*-2-benzoxacyclotetradecen-1-one sesquihydrate, $C_{18}H_{24}O_5.1.5H_2O$. There are two independent molecules in the asymmetric unit. The molecule consists of a 14-membered lactone ring fused *ortho* to a 1,3-dihydroxybenzene moiety. The crystal structure is stabilized by O—H···O hydrogen bonds. There are three water molecules filling the unit cell and forming a three-dimensional network of hydrogen bonds.

Comment

Zearalenone (Urry, Wehrmeister, Hodge & Hidy, 1966) is a common strogenic secondary metabolite produced by several species of *Fusarium*. Among a number of derivatives of zearalenone isolated from *F. roseum* (Stipanovic & Schroeder, 1975), zearalenol was found to be four times more active than zearalenone in rat uterotropic assay (Pathre & Mirocha, 1976). The present work describes the structure determination and crystal packing of the title compound.



Bond distances and angles are in agreement with the related compound α-zearalenol, reported by Watson, Zabel, Mirocha & Pathre (1982). There are two independent molecules in the asymmetric unit (denoted *A* and *B*) with almost the same conformation. This molecule consists of a phenyl ring (C16–C21) fused to a 14-membered lactone ring (C1–C10, O11, C12, C16, C21). The average C—C bond lengths of the phenyl ring are 1.395 (4) and 1.392 (4) Å for *A* and *B*, respectively. In both molecules, the phenyl ring is planar to within 0.009 (2) Å. The *trans* C1═C2 double bond is twisted out of the plane of the phenyl ring as indicated by the C2—C1—C21—C16 torsion angle [155.8 (3) and 156.7 (3)° for *A* and *B*, respectively] and the C1—C21 distance [1.483 (4) and 1.484 (4) Å for *A* and *B*, respectively], indicating some degree of conjugation. The configuration at C10 is known to be *S* with reference to zearalenone (Kuo *et al.*, 1967; Taub *et al.*, 1968). The configuration at C6 is *S*, confirming the title compound to be β-zearalenol. The torsion angles (see Table 2) for both molecules indicate similar conformation between them and those in α-zearalenol, except that the latter has an *R* configuration at C6.

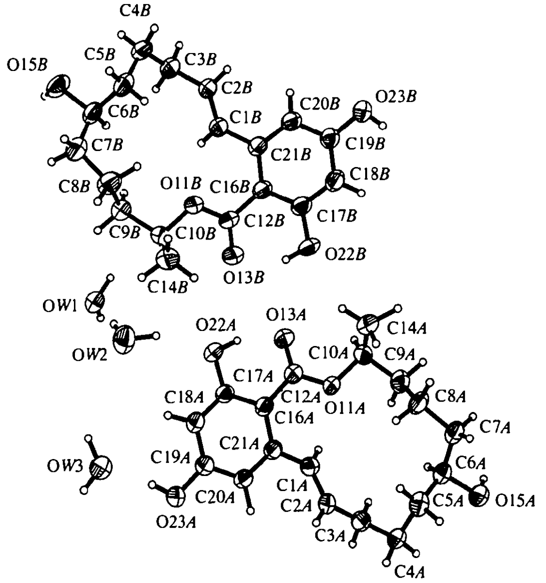


Fig. 1. The molecular structure of the title compound with the atom labelling; 50% probability displacement ellipsoids are shown.

The O—H···O hydrogen bonds are given in Table 3. The molecule contains three hydroxy groups. In both molecules the hydroxy group at C17 interacts with the carbonyl O atom located at C12, forming a strong

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† Contribution No. 1440 of the Instituto de Química, UNAM.

Acta Crystallographica Section C
ISSN 0108-2701 © 1996