C1—C9	1.455 (3)	C8—C10	1.418 (3)
C1—C11	1.406 (3)	C9—C10	1.421 (3)
C2—C3	1.441 (3)	C12—C13	1.510 (3)
C3—C4	1.343 (3)	C13—C14	1.513 (3)
C4—C10	1.427 (3)	N—H1N	0.775
C11—N—C12	125.3 (2)	C6—C7—C8	118.9 (2)
C2—C1—C9	120.8 (2)	C7—C8—C10	121.5 (2)
C2—C1—C11	118.8 (2)	C1—C9—C5	124.1 (2)
C9—C1—C11	120.4 (2)	C1—C9—C10	118.6 (2)
O—C2—C1	122.9 (2)	C5—C9—C10	117.3 (2)
O—C2—C3	119.8 (2)	C4—C10—C8	121.7 (2)
C1—C2—C3	117.3 (2)	C4—C10—C9	119.0 (2)
C2—C3—C4	121.8 (2)	C8—C10—C9	119.4 (2)
C3—C4—C10	122.4 (2)	N—C11—C1	124.4 (2)
C6—C5—C9	121.5 (2)	N—C12—C13	112.1 (2)
C5—C6—C7	121.5 (2)	C12—C13—C14	112.4 (2)
N—C12—C13—C14	173.9 (2)	O—C2—C3—C4	−178.1 (3)
C5—C9—C10—C4	179.1 (2)	C1—C9—C10—C8	−179.9 (2)
C11—N—C12—C13	107.8 (2)	C12—N—C11—C1	−173.5 (2)
C2—C1—C9—C5	−176.9 (2)	C11—C1—C9—C5	4.8 (1)
C11—C1—C9—C10	−175.6 (2)	C9—C1—C11—N	−179.6 (2)

All non-H atoms were refined by anisotropic full-matrix least squares. H atoms were treated as riding atoms with C—H = 0.95 Å except for the one involved in the intramolecular N—H···O hydrogen bond which was found from a difference Fourier map. All H atoms were included in the structure-factor calculations with isotropic displacement parameters set to 1.2 × U_{eq} of the atom to which they are bonded. Owing to the severe extinction, the reflection 100 was omitted from the least-squares refinement.

Data collection: *STADI4* (Stoe, 1995*a*). Cell refinement: *STADI4*. Data reduction: *X-RED* (Stoe, 1995*b*). Program(s) used to solve structure: *NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to refine structure: *NRCVAX*. Molecular graphics: *NRCVAX*. Software used to prepare material for publication: *NRCVAX*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KA1185). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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3,4,5,6-Tetra-*O*-benzyl-*cis*-1,2-*O*-cyclohexylidene *myo*-Inositol

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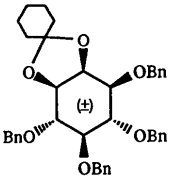
Abstract

The inositol ring in $C_{40}H_{44}O_6$ is in a chair conformation with the O atom at C2 in the expected axial position and the other five O atoms in equatorial positions. The ring is twisted with one approximate twofold axis retained through the mid-points of the C2—C3 and C5—C6 bonds.

Comment

3,4,5,6-Tetra-*O*-benzyl-*cis*-1,2-*O*-cyclohexylidene *myo*-inositol, (1), is an important intermediate in the syntheses of inositol phosphates and analogues, including *myo*-inositol 1-phosphate (Kiely, Abruscato & Baburao, 1974), *myo*-inositol 1-phosphorothioate (Baker, Billington & Gani, 1991), *myo*-inositol 2-phosphate (Billington, 1993) and *myo*-inositol 1,2-bisphosphate (Spiers *et al.*, 1996). In the presence of acid, the acetal group of (1) cleaves to give 3,4,5,6-tetra-*O*-benzyl *myo*-inositol, the 2-hydroxy position of which is more reactive than the 1-position, a selectivity which is exploited in many of the aforementioned syntheses.



(1)

The biologically important parent compound *myo*-inositol has been analysed by X-ray diffraction, both in the absence (Rabinowitz & Kraut, 1964) and presence of two molecules of water (Lomer, Miller & Beevers, 1963). Both determinations showed the cyclohexane ring to exist in the chair conformation with one of the six hydroxyl groups axial and the others equatorial (1*a*/5*e*). The distortion of the ring from a perfect chair was small in both cases; this was also observed in the fully protected derivatives, 1,2,3,4,5,6-

hexa-*O*-acetyl *myo*-inositol (Abboud, Simonsen, Voll & Younathan, 1990) and (±)-3,4-di-*O*-acetyl-1,2,5,6-tetra-*O*-benzyl *myo*-inositol (Steiner, Hinrichs, Saenger & Gigg, 1993). Ion binding to *myo*-inositol by magnesium chloride (Blank, 1973) and calcium bromide (Cook & Bugg, 1973) as hydrate complexes has been shown to impose more noticeable ring distortion but still retain the expected (1*a*/5*e*) conformation. On the other hand, the dodecasodium salt of *myo*-inositol hexakisphosphate (phytic acid) adopts the unusual (5*a*/1*e*) conformation (Blank, Pletcher & Sax, 1975), the phosphates being stabilized by bridging sodium ions and hydrogen-bonded water molecules. In contrast, both *myo*-inositol 2-phosphate monohydrate (Yoo, Blank, Pletcher & Sax, 1974) and *myo*-inositol 1,2,3-trisphosphate (Spiers, Freeman & Schwalbe, 1995) were found to exist in slightly distorted (1*a*/5*e*) chair conformations.

The inositol ring of compound (1) is in a distorted chair conformation with the O atom at C2 (Fig. 1) in the expected axial position and the other five O atoms in equatorial positions. All the inositol C—C and C—O bond lengths (Table 2) are comparable with those of *myo*-inositol (Rabinowitz & Kraut, 1964). However, four of the six inositol ring angles (Table 2) exceed expected values by >1° [*myo*-inositol has a mean angle of 110.7° (Rabinowitz & Kraut, 1964) and the perfect chair form was estimated to have an angle of 111° (Bucourt, 1974)] with the largest deviation at position C02. The O08—C02—C01—O09 torsion angle of 38.6 (3)° (this would normally approach 60°) shows that the inositol O atoms at the *cis* ring junction have moved closer together to accommodate the acetal linkage. The asymmetry parameters of the inositol ring (Duax & Norton, 1975) are: $\Delta C_s(1)$ = 9.9 (3), $\Delta C_s(2)$ = 5.5 (3), $\Delta C_s(3)$ = 15.4 (3), $\Delta C_2(1–2)$ = 3.1 (4), $\Delta C_2(2–3)$ = 14.8 (4), $\Delta C_2(3–4)$ = 17.9 (4)°. The inositol ring is twisted with one approximate twofold axis retained [$\Delta C_2(2–3)$]. The distances of inositol ring atoms from their best-fit plane [C01 −0.143 (3), C02 0.131 (3), C03 −0.191 (3), C04 0.271 (3), C05 −0.287 (3), C06 0.219 (3) Å] confirm the ring distortion, showing that atoms C02 and C03 are pulled in much closer to the plane, and that C05 and C06 are pushed further away from the plane.

The cyclohexylidene ring is in the chair conformation with ring and torsion angles slightly deviating from those of the ideal form (Bucourt, 1974). The slight distortion is thought to be compensation for the acetal linkage.

The acetal five-membered ring adopts an envelope conformation; C02 lies 0.600 (5) Å below the plane through the other atoms [all deviations 0.000 (2) Å], with $\Delta C_s(2)$ = 1.9 (3)°.

The four *O*-benzyl groups each have three bonds about which rotation may occur and consequently they exhibit conformational flexibility, as shown in the crystal structure of (±)-3,4-di-*O*-acetyl-1,2,5,6-tetra-*O*-benzyl *myo*-inositol (Steiner, Hinrichs, Saenger & Gigg, 1993). The benzyl groups have bond distances and angles which are comparable with one another. The CH_2 groups at C40 and C33 are orientated towards C05, and the CH_2 group at C26 is orientated towards C04. The acetal linkage creates space which allows the CH_2 group at C13 to orientate towards C02 and this reduces crowding with the other benzyl groups. All phenyl groups are antiperiplanar with respect to the inositol C—O bond which suggests a concerted orientation for these groups, and their phenyl planes are synclinal with respect to the O—CH_2 bonds.

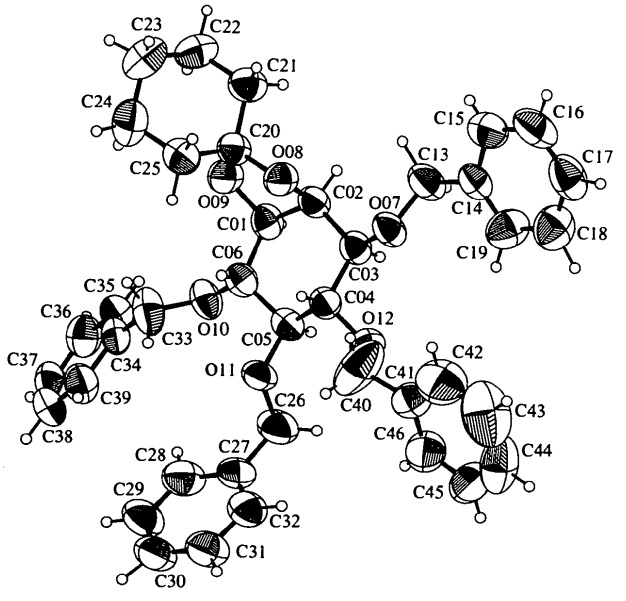


Fig. 1. The title compound (1), showing the labelling scheme for the non-H atoms. Ellipsoids are drawn at the 50% probability level.

Experimental

The title compound (1) was prepared in a two-step procedure from *myo*-inositol, using the method of Baker, Billington & Gani (1991). The first step was the reaction of *myo*-inositol with cyclohexanone to give (±)-*cis*-1,2-*O*-cyclohexylidene *myo*-inositol; subsequent benzylation of this intermediate gave (1) which was recrystallized from chloroform and hexane.

Crystal data

$C_{40}H_{44}O_6$
M_r = 620.75
Monoclinic
$P2_1/c$
a = 10.608 (3) Å
b = 19.147 (6) Å
c = 17.448 (5) Å
β = 107.22 (2)°
V = 3385.0 (17) Å^3
Z = 4
D_x = 1.218 Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 9.78–13.96°
μ = 0.081 mm^{-1}
T = 293 (2) K
Rectangular block
0.48 × 0.43 × 0.35 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.0261$
$\omega/2\theta$ scans	$\theta_{max} = 24.97°$
Absorption correction: none	$h = -12 \rightarrow 5$
9021 measured reflections	$k = -22 \rightarrow 0$
5893 independent reflections	$l = -20 \rightarrow 20$
2702 observed reflections $[I > 2\sigma(I)]$	3 standard reflections frequency: 120 min intensity decay: 4.4%

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max} = 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.0511$	$\Delta\rho_{max} = 0.207$ e Å^{-3}
$wR(F^2) = 0.1513$	$\Delta\rho_{min} = -0.167$ e Å^{-3}
$S = 1.005$	Extinction correction: none
5883 reflections	Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
565 parameters	
$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 1.6552P]$ where $P = (F_o^2 + 2F_c^2)/3$	

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

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

	x	y	z	U_{eq}
C01	0.1950 (3)	0.4067 (2)	0.1399 (2)	0.0631 (9)
C02	0.1825 (3)	0.3286 (2)	0.1487 (2)	0.0602 (9)
C03	0.0454 (3)	0.2984 (2)	0.1145 (2)	0.0612 (9)
C04	−0.0594 (3)	0.3422 (2)	0.1346 (2)	0.0589 (8)
C05	−0.0522 (3)	0.4176 (2)	0.1086 (2)	0.0614 (9)
C06	0.0811 (3)	0.4484 (2)	0.1531 (2)	0.0619 (9)
O07	0.0350 (2)	0.22909 (11)	0.14124 (14)	0.0680 (6)
O08	0.2283 (2)	0.32045 (11)	0.23369 (13)	0.0642 (6)
O09	0.3159 (2)	0.42081 (11)	0.20119 (14)	0.0695 (6)
O10	0.0896 (2)	0.51911 (11)	0.12909 (13)	0.0721 (7)
O11	−0.1507 (2)	0.45740 (11)	0.12920 (13)	0.0701 (7)
O12	−0.1860 (2)	0.31307 (12)	0.09624 (13)	0.0684 (6)
C13	0.1153 (4)	0.1799 (2)	0.1165 (3)	0.0846 (12)
C14	0.0594 (4)	0.1076 (2)	0.1191 (2)	0.0669 (9)
C15	0.1412 (5)	0.0543 (3)	0.1590 (3)	0.0935 (14)
C16	0.0929 (6)	−0.0142 (2)	0.1571 (3)	0.103 (2)
C17	−0.0356 (6)	−0.0261 (3)	0.1145 (3)	0.099 (2)
C18	−0.1168 (6)	0.0273 (3)	0.0782 (3)	0.1025 (14)
C19	−0.0684 (5)	0.0935 (2)	0.0808 (3)	0.0923 (13)
C20	0.3378 (3)	0.3664 (2)	0.2608 (2)	0.0623 (9)
C21	0.4678 (4)	0.3300 (2)	0.2656 (3)	0.0758 (11)
C22	0.5849 (4)	0.3767 (3)	0.3007 (3)	0.0898 (13)
C23	0.5854 (5)	0.4038 (3)	0.3815 (3)	0.108 (2)
C24	0.4579 (5)	0.4425 (3)	0.3763 (3)	0.106 (2)
C25	0.3389 (4)	0.3960 (2)	0.3408 (3)	0.0794 (11)
C26	−0.2576 (5)	0.4806 (3)	0.0642 (3)	0.0923 (14)
C27	−0.3356 (4)	0.5305 (2)	0.0980 (2)	0.0758 (10)
C28	−0.2956 (4)	0.5989 (2)	0.1134 (3)	0.0901 (13)
C29	−0.3616 (5)	0.6443 (2)	0.1496 (3)	0.0974 (14)
C30	−0.4694 (4)	0.6216 (2)	0.1702 (3)	0.0924 (13)
C31	−0.5108 (5)	0.5543 (2)	0.1544 (3)	0.0946 (14)
C32	−0.4440 (5)	0.5093 (2)	0.1188 (3)	0.0897 (13)
C33	0.0955 (7)	0.5681 (2)	0.1909 (3)	0.0921 (14)
C34	0.0923 (4)	0.6409 (2)	0.1587 (2)	0.0654 (9)
C35	0.1705 (4)	0.6621 (2)	0.1131 (2)	0.0719 (10)
C36	0.1675 (5)	0.7306 (2)	0.0869 (3)	0.0823 (12)
C37	0.0858 (5)	0.7773 (2)	0.1061 (3)	0.0839 (13)
C38	0.0067 (5)	0.7578 (2)	0.1499 (3)	0.0851 (12)
C39	0.0108 (4)	0.6900 (2)	0.1770 (3)	0.0804 (12)
C40	−0.2581 (5)	0.2979 (3)	0.1493 (3)	0.147 (2)
C41	−0.3743 (4)	0.2523 (2)	0.1101 (2)	0.0754 (10)
C42	−0.3801 (6)	0.1874 (3)	0.1382 (3)	0.134 (2)
C43	−0.4922 (10)	0.1463 (3)	0.1083 (5)	0.166 (3)
C44	−0.5940 (7)	0.1727 (4)	0.0511 (4)	0.128 (2)
C45	−0.5895 (5)	0.2359 (4)	0.0230 (3)	0.115 (2)
C46	−0.4803 (5)	0.2765 (2)	0.0528 (3)	0.0965 (13)

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

C01—C06	1.522 (5)	C03—O07	1.421 (4)
C01—O09	1.431 (4)	C04—O12	1.425 (4)
C02—C01	1.513 (4)	C05—C04	1.522 (4)
C02—O08	1.426 (4)	C05—O11	1.423 (4)
C03—C02	1.515 (5)	C06—C05	1.517 (5)
C03—C04	1.514 (4)	C06—O10	1.428 (4)
C01—C02—C03	116.1 (3)	C04—C03—C02	112.5 (3)
C02—C01—C06	114.0 (3)	C05—C06—C01	112.3 (3)
C03—C04—C05	110.6 (3)	C06—C05—C04	109.8 (3)
C01—C06—C05—C04	57.5 (4)	C03—C02—C01—C06	39.6 (4)
C02—C01—C06—C05	−46.4 (4)	C04—C03—C02—C01	−43.6 (4)
C02—C03—C04—C05	54.1 (4)	C06—C05—C04—C03	−61.5 (4)

All H-atom positions were found in a difference synthesis and were refined freely, except for one benzyl group which had its H atoms placed in calculated positions to ride on attached atoms, with group isotropic displacement parameters. This benzyl group has high thermal motion.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *DATRED* (Brookhaven National Laboratory & Birmingham University, 1986). Program(s) used to solve structure: *MULTAN*84 (Main, Germain & Woolfson, 1984). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CF1070). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Maleimide

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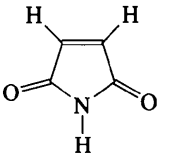
Abstract

The triclinic unit cell of maleimide (1*H*-pyrrole-2,5-dione, $C_4H_3NO_2$), contains eight molecules which form four hydrogen-bonded dimers. Each dimer comprises a planar tricyclic ring system.

Comment

Maleimide, (I), is a reactive vinyl monomer used in free-radical-initiated polymerizations (Kirk–Othmer Encyclopaedia, 1983). A variety of polymers used for high-temperature aerospace applications are based on substituted cyclic five-membered imide rings. In particular, the polymer obtained from methylene dianiline bismaleimide is one of the most commonly used materials for these applications (Wilson, 1987). The maleimide group is also present in the antibiotic showdomycin (Neidle, Kaye & Reese, 1990) and antitumour activity has been shown by *N*-glycinylmaleimide and its copolymers (Gam, Jeong, Lee, Ha & Cho, 1995). Maleimide compounds are also used in biochemical conjugations such as selective biotinylation of sulfhydris (Dojindo Laboratories, 1996). The structures of compounds similar to maleimide such as maleic anhydride (Marsh, Ubell & Wilcox, 1962) in which the endocyclic N atom is replaced by an O atom, and succinimide (Mason, 1961) in which the double bond is replaced by a single bond, were examined decades ago. However, X-ray analysis of maleimide required a low-temperature (150 K) study and rapid data collection to prevent decay of the crystal. In this study, the mosaicity of the crystal was also somewhat higher than normal (1.9° compared to 0.5–1.2°) and cell dimensions were obtained with some difficulty. Other triclinic and monoclinic cells derived from the experimental cell dimensions were examined with the program *LEPAGE* (Spek, 1988), but the experimental cell was the only one which resulted in a structure solution. Pseudosymmetry relating to a twofold axis is present between the atoms of molecules *A* and *D* and between those of *B* and *C*. This is shown by the average *y* coordinate of corresponding atom pairs which in each case is very close to 0.25.



(I)

In the crystal, pairs of maleimide molecules are linked together to form planar tricyclic dimers (Fig. 1) by pairs of intermolecular N1—H···O1 hydrogen bonds. Molecule *A* links to molecule *C* and molecule *B* links to molecule *D*. The centre ring so formed contains eight atoms including the two H atoms. The dimers pack in sheets parallel to the *b* axis with the hydrogen bonding confined to each pair of dimers. In each molecule, the C—O bonds are longer where the O atom acts as an acceptor [C1—O1 range 1.214 (7)–1.235 (7) Å] than where it has no hydrogen-bonding role [C4—O2 range 1.190 (7)–1.221 (7) Å]. The O···N distances range from 2.851 (7)–2.917 (7) Å, the O···H distances from 1.98–2.05 Å and the N—H···O angles from 167–171°. (The N—H distances were fixed at 0.88 Å.) The C=C double bond [1.301 (8)–1.322 (8) Å] is normal and there is little evidence for any other tautomeric form. The diketo tautomer of maleimide has also been shown to be the most stable form in both the gas and solution phase (Acker, Hofmann & Cimiraglia, 1994).

Each of the four molecules (including H atoms) is approximately planar with deviations of atoms from the mean least-squares planes ranging from −0.025 (4) to 0.025 (4) Å for *A*, −0.030 (4) to 0.033 (3) Å for *B*, −0.048 (3) to 0.055 (4) Å for *C* and −0.016 (3) to 0.016 (6) Å for *D*. The dimers are also somewhat planar with atom deviations from the best mean planes ranging from −0.145 (5) to 0.091 (5) Å for *A*/*C* and from −0.116 (5) to 0.100 (4) Å for *B*/*D*. The two dimers pack