Deciphering the hydrogen-bonding scheme in the crystal structure of triphenylmethanol: a tribute to George Ferguson and co-workers

Tomasa Rodríguez Tzompantzi,[a] **Aldo Guillermo Amaro Hernández,**[a] **Rosa Luisa Meza-León**[a] **and Sylvain Bernès**[b]*

[a]Facultad de Ciencias Químicas, Benemérita Universidad Autónoma de Puebla, Av. San Claudio y 18 Sur, 72570 Puebla, Pue., Mexico, and [b]Instituto de Física, Benemérita Universidad Autónoma de Puebla, Av. San Claudio y 18 Sur, 72570 Puebla, Pue., Mexico. *Correspondence e-mail: sylvain_bernes@hotmail.com

The crystal structure of triphenylmethanol, $C_{19}H_{16}O$, has been redetermined using data collected at 295 and 153 K, and is compared to the model published by Ferguson *et al.* over 25 years ago [Ferguson *et al.* (1992). *Acta Cryst.* C**48**, 1272–1275] and that published by Serrano-González *et al.*, using neutron and X-ray diffraction data [Serrano-González *et al.* (1999). *J. Phys. Chem. B*, **103**, 6215–6223]. As predicted by these authors, the hydroxy groups are involved in weak intermolecular hydrogen bonds in the crystal, forming tetrahedral tetramers based on the two independent molecules in the asymmetric unit, one of which is placed on the threefold symmetry axis of the $R\bar{3}$ space group. However, the reliable determination of the hydroxy H-atom positions is difficult to achieve, for two reasons. Firstly, a positional disorder affects the full asymmetric unit, which is split over two sets of positions, with occupancy factors of *ca* 0.74 and 0.26. Secondly, all hydroxy H atoms are further disordered, either by symmetry, or through a positional disorder in the case of parts placed in general positions. We show that the correct description of the hydrogen-bonding scheme is possible only if diffraction data are collected at low temperature. The prochiral character of the hydrogen-bonded tetrameric supramolecular clusters leads to enantiomorphic three-dimensional graphs in each tetramer. The crystal is thus a racemic mixture of ^{sup}S and ^{sup}R motifs, consistent with the centrosymmetric nature of the $R\bar{3}$ space group.

1. Introduction

The hydroxy group is known as one of the most efficient nodes for the formation of hydrogen bonds, as a consequence of the polarization of the O—H bond, and also because it can behave both as donor and acceptor for building intra- or intermolecular bonds. In this context, the emblematic donor–acceptor molecule is water, and many compounds have been crystallized as hydrates, in which the lattice water molecules contribute to a significant part of the crystal free energy (Batsanov, 2018); currently, almost 13% of the structures deposited in the Cambridge Structural Database are hydrates (CSD, Version 5.40, updated February 2019; Groom *et al.*, 2016). The situation is a bit less favourable in the case of alcohols (RO—H), especially for tertiary alcohols having the hydroxy group surrounded by bulky hydrocarbon groups. For example, three hydrates for *tert*-butanol, $(CH_3)_3COH$, have been successfully characterized [namely the dihydrate and heptahydrate (Mootz & Stäben, 1993), and the decahydrate (Dobrzycki, 2018)], while tri-*tert*-butylmethanol, $[(CH_3)_3C]_3$-COH, has probably never been crystallized, although it has been studied in the solid state (Malarski, 1974). Although this
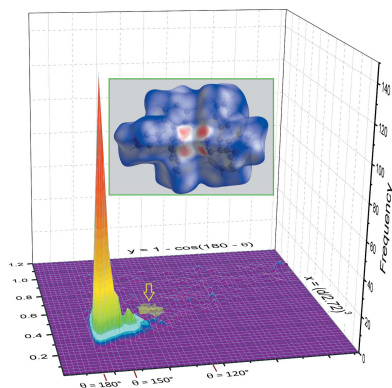

OPEN ACCESS

Table 1
Experimental details.

For both determinations: $C_{19}H_{16}O$, $M_r = 260.32$, trigonal, $R\overline{3}{:}H$, $Z = 24$. Experiments were carried out with Ag $K\alpha$ radiation ($\lambda = 0.56083$ Å) using a Stoe Stadivari diffractometer. Absorption was corrected for by multi-scan methods (*X-AREA*; Stoe & Cie, 2018). Refinement was on 483 parameters. H-atom parameters were constrained.

	153 K data	295 K data
Crystal data		
Temperature (K)	153	295
a, c (Å)	19.1399 (5), 26.7399 (9)	19.3309 (8), 26.8542 (11)
V (Å^3)	8483.4 (5)	8690.5 (8)
μ (mm^{-1})	0.05	0.05
Crystal size (mm)	$0.33 \times 0.29 \times 0.25$	$0.38 \times 0.33 \times 0.33$
Data collection		
T_{min}, T_{max}	0.419, 1.000	0.558, 1.000
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	99452, 4399, 2222	72080, 4523, 1656
R_{int}	0.069	0.108
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.653	0.653
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.167, 1.00	0.063, 0.242, 0.99
No. of reflections	4399	4523
No. of restraints	72	279
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.14	0.11, −0.14

Computer programs: *X-AREA* (Stoe & Cie, 2018), *SHELXT2018* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *XP* in *SHELXTL-Plus* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

molecule is stable, it is not able to form stabilizing inter-molecular O—H···O hydrogen bonds, because of the steric hindrance of the three *tert*-butyl groups surrounding the OH donor group (Majerz & Natkaniec, 2006).
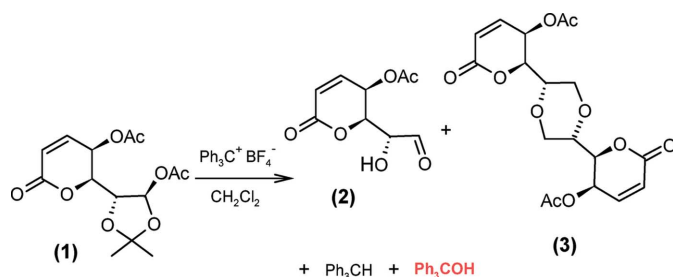

Triphenylmethanol
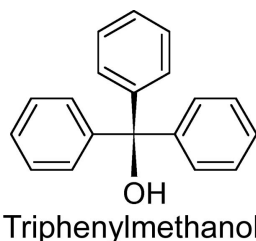
The case of triphenylmethanol, $(C_6H_5)_3COH$, should be intermediate between *tert*-butanol and tri-*tert*-butylmethanol, since it can be used as a clathrate host for methanol (Weber *et al.*, 1989), and may be hydrogen bonded to a water molecule (Batisai *et al.*, 2016), dimethyl sulfoxide, dimethylformamide (Eckardt *et al.*, 1999) or $Ph_3P{=}O$ (Steiner, 2000). Indeed, unsolvated triphenylmethanol can be easily crystallized from

Figure 1
Synthetic step from which triphenylmethanol was crystallized. Note that product (**2**) was not obtained.

benzene or ethanol, affording large well-shaped clear colour-less single crystals. However, these crystals are always weakly diffracting samples, as a consequence of a severe structural disorder (*vide infra*). The resulting ratio of observed to measured reflections is then quite low, which, in turn, makes the refinement very difficult. First attempts to refine a reasonable model failed (Weber *et al.*, 1989), and it was only in 1992 that the crystal structure was published (Ferguson *et al.*, 1992), based on room-temperature intensities measured on a CAD-4 diffractometer, with Mo $K\alpha$ radiation. 2467 unique reflections were used, of which 41% were observed [$I > 2.5\sigma(I)$], and the structure was refined with a structural motif described as a 'hydrogen-bonded pyramidal tetramer which is disordered (71/29) about two interpenetrating sites'. The refinement was of limited accuracy and converged to $R = 0.083$ and $wR = 0.068$ with rigid idealized phenyl rings for all molecules, and isotropic atoms in the minor-disordered part of the asymmetric unit (253 variable parameters).

Although the structure reported by Ferguson *et al.* was incomplete, since hydroxy H atoms could not be located, the *savoir-faire* used by this team is quite impressive. They were able to solve and refine this challenging disordered structure, while others probably gave up by arguing that crystals were badly twinned. Above all, they did not attempt to over-inter-pret their data, and were aware that hydroxy H atoms were very imprecisely determined in their X-ray diffraction experiment. However, they indirectly recognized and des-cribed the presence of a weak hydrogen-bonding scheme, reflected in intermolecular O···O contacts.

In 1999, Serrano-González *et al.* (1999) published a more elaborate article, focussed on the characterization of the hydrogen-bonding arrangement in triphenylmethanol, using neutron ($T = 100$ K) and X-ray diffraction data ($T = 113$ and

293 K), as well as solid-state ^{13}C NMR spectroscopy. A reliable structure based on neutron diffraction data was obtained, showing that each independent OH group has the H atom disordered over three sites. This model was then a suitable starting point for the refinement of X-ray structures, both at 113 and 293 K. Unfortunately, the final atomic coordinates were never deposited in the CSD, and there is no CIF available as supporting information. Fractional coordinates are tabulated, however, for X-ray refinements, H atoms are missing. Moreover, even using the favourable neutron scattering length for the protium nucleus, it was not possible to complete the structure. As stated in this article 'The hydroxy hydrogens of the minor tetramer could not be located from the difference Fourier map, and these hydrogen atoms were inserted in calculated positions based on those determined [. . .] for the major tetramer'.

We have now completed these works, using X-ray data collected at room temperature and low temperature with the Ag $K\alpha$ radiation, revealing the accurate localization of the hydroxy H atoms in the disordered structure. A comprehensive insight into the hydrogen-bonding scheme that held together the tetrameric clusters is now afforded.

2. Experimental

2.1. Synthesis and crystallization

We obtained triphenylmethanol as a by-product during the oxidative hydrolysis of the diacetylated compound (**1**), following a method proposed by Barton *et al.* (1972) (Fig. 1). Compound (**1**) (0.100 g, 0.318 mmol) and triphenylcarbenium

tetrafluoroborate (0.099 g, 0.380 mmol) were mixed in dry CH_2Cl_2 (20 ml) and stirred for 15 min at room temperature. A saturated solution of $NaHCO_3$ was then added (10 ml), the organic phase dried over Na_2SO_4 and the crude product chromatographed (silica gel, hexane–ethyl acetate, 90:10 *v/v*). The expected hydroxy aldehyde (**2**) was not observed, and the dimer (**3**) was isolated instead, mixed with triphenylmethane and triphenylmethanol. It was not possible to separate (**3**) and triphenylmethanol by chromatography, whereby the mixture was purified by crystallization in hexane–ethyl acetate (95:5 *v/ v*), affording large single crystals of triphenylmethanol [yield 30 mg; m.p. 431–433 K, literature 434–435 K (Zeiss & Tsutsui, 1953)]. ^{1}H NMR (CDCl$_3$/TMS, 300 MHz): δ 2.8 (*s*, 1H, OH), 7.30 (*s*, 15H, Ph). ^{13}C NMR (CDCl$_3$/TMS, 75 MHz): δ 99.8 (C—OH), 127.2, 127.9, 146.8 (Ph).

2.2. Refinements

Crystal data, data collection and structure refinement details are summarized in Table 1 for the two different crystals obtained from a single crystallization batch, but diffracted at different temperatures, *i.e.* 153 and 295 K. The disorder in the asymmetric unit was solved using the low-temperature data set, and all phenyl rings were restrained to be flat, with standard deviations of 0.1 Å^3. Additionally, the phenyl rings in the minor part (molecules *C* and *D*) were restrained to have 1,3 distances similar to those in the corresponding rings of the disordered counterpart (molecules *A* and *B*), within standard deviations of 0.02 Å. H atoms in the phenyl rings were placed in idealized positions and refined as riding to their carrier C atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. Hydroxy H atoms were
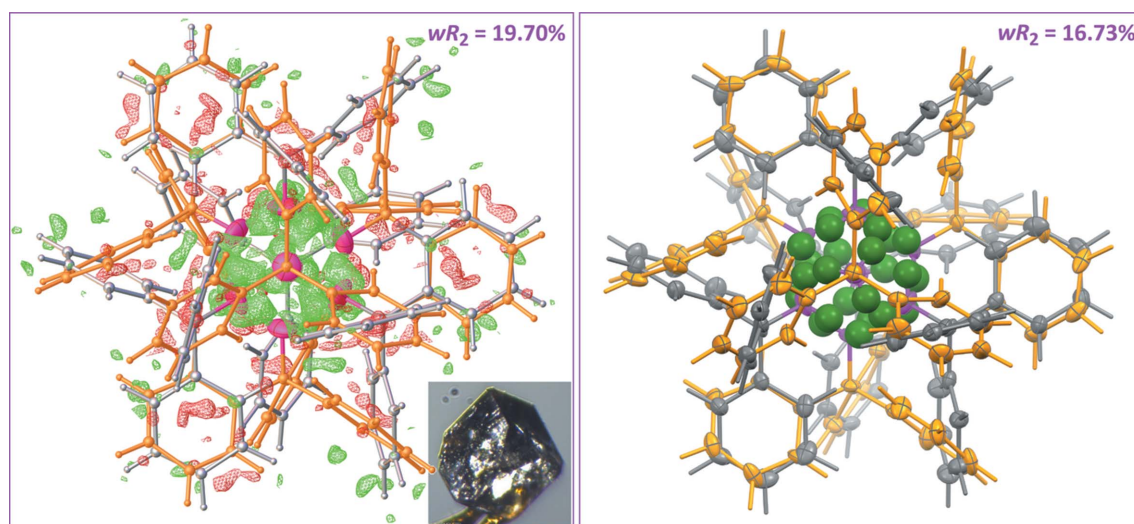
Figure 2
(Left) Difference electron-density map computed using low-temperature data, after refining the full disordered model but omitting hydroxy H atoms. Grey molecules correspond to the main part *A/B* (occupancy 0.74) and gold molecules to the minor part *C/D* (occupancy 0.26); hydroxy O atoms are represented with magenta ellipsoids. Two tetramers are displayed in a projection along the threefold crystallographic axis. The difference map is plotted at the 0.33 e Å^{-3} level (green wire for $\Delta\rho > 0$ and red wire for $\Delta\rho < 0$; Dolomanov *et al.*, 2009). Note how most of the positive residuals are concentrated within the cavity delimited by the eight clustered O atoms. The inset is the crystal used for data collection. Note the triangular face on the top of the crystal, corresponding to the (003) face. (Right) Final model, including 24 disordered hydroxy H atoms, shown as green spheres with a radius corresponding to 33% of the van der Waals radius. All C and O atoms are displayed with displacement ellipsoids at the 20% probability level (*Mercury*; Macrae *et al.*, 2008).

found in a difference map (Fig. 2, left) and refined with $U_{iso}(H) = 1.5U_{eq}(O)$. Atoms H1A and H1C are disordered by symmetry, and their site occupancies were fixed as one-third of the occupancy of the part to which they belong. The hydroxy H atoms for molecules in general positions are disordered over sites H1BA, H1BB and H1BC for molecule B, and H1DA, H1DB and H1DC for molecule D, and the occupancy for each site was also fixed as one-third of the occupancy of the part to which it belongs. The geometry of the C—O—H groups was first restrained to a sensible target, by restraining distances to O—H = 0.85 (1) Å and C···H = 1.93 (2) Å in molecules A and C; for molecules B and D, the applied restraints were O—H = d, H···H = $(8/3)^{1/2} \times d$ and C···H = $2.27 \times d$, where d is a common free variable. Standard

deviations for these restraints were 0.02, 0.03 and 0.03 Å, respectively. After convergence, the positions of all hydroxy H atoms were fixed, and these atoms were refined as riding on their carrier O atoms. The final model for the complete structure at 153 K was refined against data collected at 295 K, with an extra restraint: in the minor-disordered part (molecules C and D), rigid-bond restraints were applied with standard deviations of 0.004 Å for the 1,2 and 1,3 distances (Thorn et al., 2012; Sheldrick, 2015b).

3. Results and discussion

The asymmetric unit of the trigonal cell includes two disordered parts with site-occupancy factors converging at 153 K
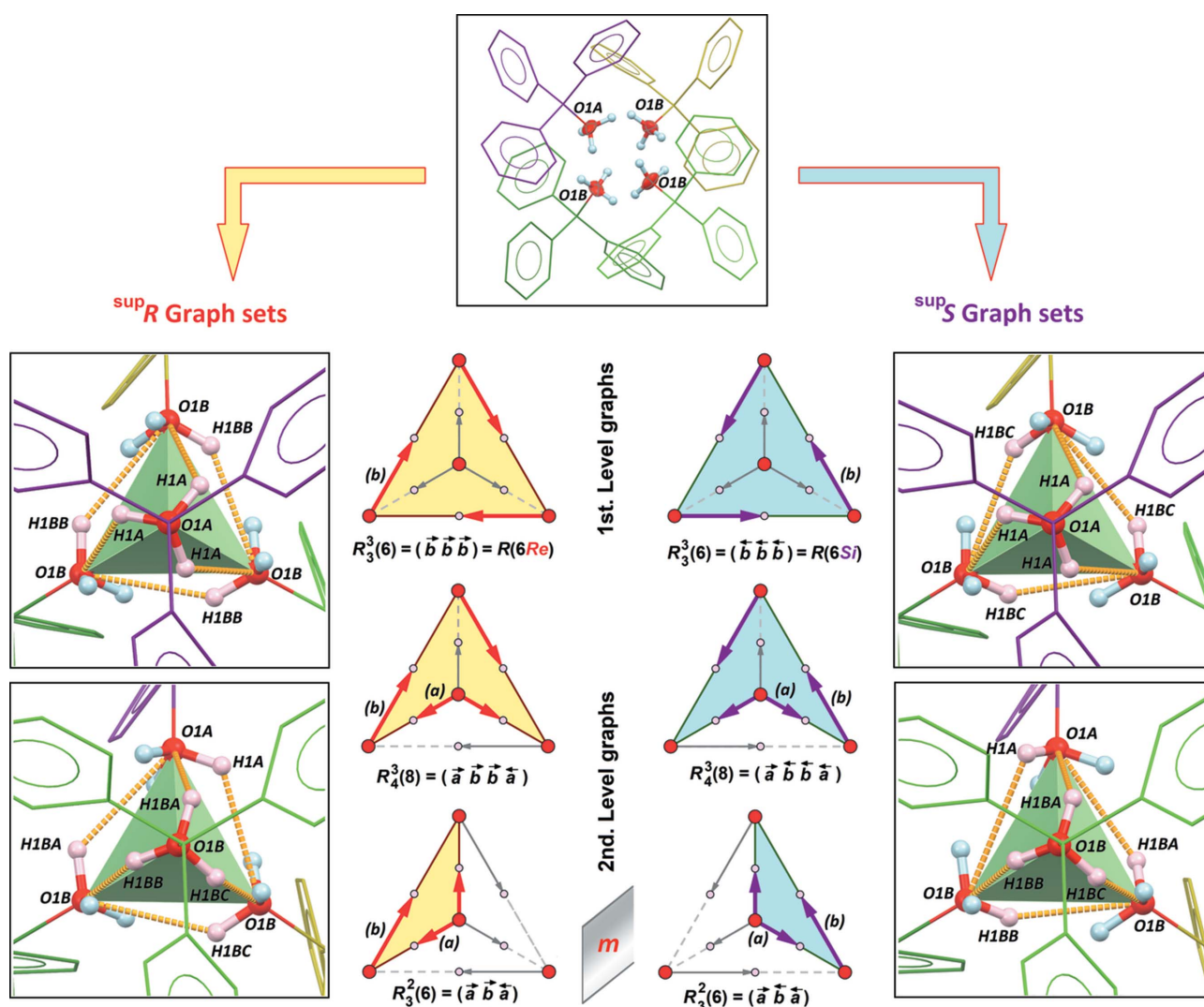
Figure 3
Hydrogen-bonding schemes in the tetramer formed by A/B molecules. The top figure shows the arrangement of the four molecules and the 12 hydroxy H-atom sites. The left and right panels represent right- (^{sup}R) and left-handed (^{sup}S) supramolecular clusters, respectively. The first figure is oriented down the crystallographic threefold axis and the other is oriented down a noncrystallographic threefold axis. Each cluster comprises six hydrogen bonds (dashed gold bonds), involving six H-atom sites (pink H atoms). Topological graphs $G(4,6)$ for supramolecular clusters based on O—H···O hydrogen bonds are represented in the centre. Nodes are represented as red balls (O atoms). Arrows forming a ring $R_d^a(n)$ are stacked over O—H covalent bonds and oriented in the direction $d \rightarrow a$, where d is the donor and a the acceptor for a hydrogen bond. Arrows involved in a ring are shown in bold, while those not participating in a ring are greyed out. Polygons delimited by R rings in the 2-space are coloured yellow and blue for ^{sup}R and ^{sup}S clusters, respectively, and rings in the projection plane are read clockwise in all cases. For the first-level graphs, Re stands for $Rectus$ and Si for $Sinister$. Note that all figures on the left are mirror images of the figures on the right, including descriptors of the R rings.

Table 2
Hydrogen-bond geometry (Å, °) for the 153 K data.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1A-H1A\cdots O1B$	0.85	2.33	2.869 (3)	121
$O1B-H1BA\cdots O1A$	0.84	2.27	2.869 (3)	129
$O1B-H1BB\cdots O1B^i$	0.82	2.21	2.869 (3)	138
$O1B-H1BC\cdots O1B^{ii}$	0.86	2.24	2.869 (3)	130
$O1C-H1C\cdots O1D$	0.85	2.22	2.856 (7)	131
$O1D-H1DA\cdots O1C$	0.84	2.24	2.856 (7)	131
$O1D-H1DB\cdots O1D^{ii}$	0.82	2.38	2.951 (8)	127
$O1D-H1DC\cdots O1D^i$	0.85	2.33	2.951 (8)	131

Symmetry codes: (i) $-y + 1, x - y, z$; (ii) $-x + y + 1, -x + 1, z$.

towards 0.7436 (17) (molecules A and B hereafter) and 0.2564 (17) (molecules C and D hereafter), close to the occupancies reported by Ferguson *et al.* of 0.71 and 0.29. Each part contains two independent molecules, one of which has the σ C—O bond lying on the threefold axis in the space group $R\bar{3}$, while the other is located in a general position. The arrangement of these four disordered molecules generates overlapped phenyl rings in the asymmetric unit, making the refinement of displacement parameters a tedious task (see §2.2). However, the molecular structure based on data collected at 153 K can be considered as satisfactory, although the refinement was carried out with restrained geometry for the phenyl rings. The refinement based on data collected at 295 K is not as easy, since the scattering power of the crystal decreases dramatically: the fraction of observed data [$I/\sigma(I) > 2$] drops from 50% at 153 K to 36% at 295 K. However, the structure is essentially unmodified, and occupancies for the disordered parts refined to 0.761 (3) and 0.239 (3). At both temperatures, all non-H atoms could be refined anisotropically (see Fig. 2, right), after which phenyl H atoms were placed in idealized positions.

The localization of the hydroxy H atoms was far more complex. A difference map using room-temperature data is useless, in contrast to the map computed with data collected at low temperature. At 153 K, most of the positive residuals are found close to the O atoms (Fig. 2, left), allowing the determination of sensible coordinates for H atoms disordered by symmetry (H1A and H1C for molecules A and C in special positions). At this point, the highest residuals are found close to O1B, forming a tetrahedral geometry with O1B; although molecule B is located in a general position, the O—H group emulates the disorder imposed by symmetry in molecule A (see top inset in Fig. 3). The same situation is repeated for molecule D, with much smaller residuals because this molecule belongs to the minor part of the disordered asymmetric unit. Ultimately, all the molecules in the crystal have their hydroxy H atoms disordered over three sites, and once the asymmetric unit is expanded to tetramers, eight independent molecules are clustered in such a way that the cavity delimited by eight O atoms is filled with 24 sites for disordered hydroxy H atoms (Fig. 2, right). Each C—O—H group can also be seen as a rigid group rotating about its C—O axis, producing for the H atom an electron density smeared out over a ring; nevertheless, the free rotation should be hindered through the formation of weak hydrogen bonds (Schröder *et al.*, 2004). Such a description would be consistent with ^{2}H NMR spectroscopy experiments carried out on Ph$_3$COD, showing that each hydroxy group is dynamic by rotation about the C—OD bond, on the 10^{-3} to 10^{-8} s time scale (Aliev *et al.*, 1998).

All OH groups behave as donor groups for intermolecular O—H$\cdots$O hydrogen bonds. For the main part A/B, with occupancy = 0.74, three B molecules placed close to the threefold axis are connected to form an $R_3^3(6)$ ring, corresponding to a first-level graph with H1BB as donor (Table 2, entry 3). This motif is repeated with H1BC (Table 2, entry 4), however, if the crystal orientation is preserved, this ring motif is enantiomorphic with the previous one. Finally, the third disordered site for the hydroxy H atom, H1BA, is engaged in a second-level graph with O1A as acceptor (Table 2, entry 2), giving a ring motif $R_3^2(6)$. Site O1A also serves as a donor, forming three symmetry-equivalent O1A—H1$A\cdots$O1B hydro-
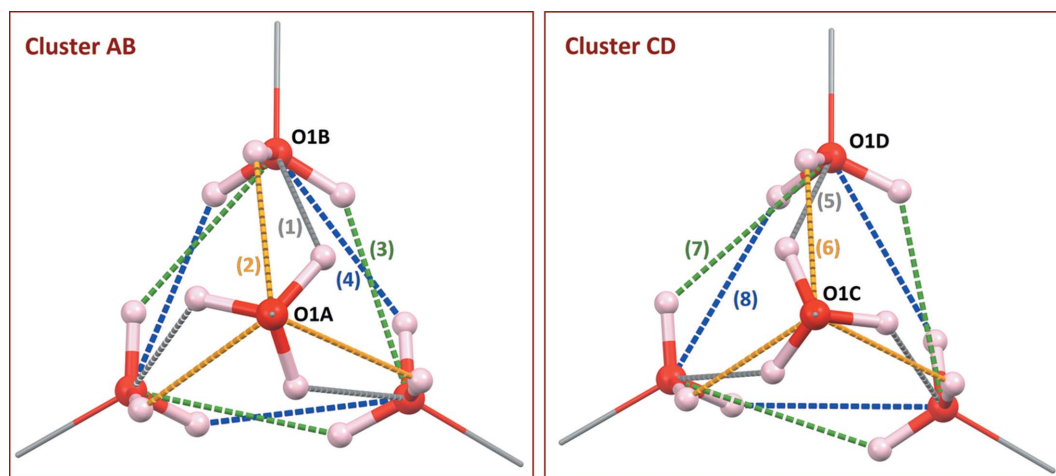
Figure 4
Complete set of hydrogen bonds, represented as dashed lines, in the tetramer formed by molecules A and B (left), and in the tetramer formed by molecules C and D (right). Figures are oriented down the crystallographic threefold axis. Labels (1)$\cdots$(8) on hydrogen bonds indicate the entry in Table 2. Each cluster has four independent bonds, affording 12 bonds for the tetramer, consistent with the C_3 point symmetry of the tetramer. These figures can be compared to the model published in 1999 (see Fig. 4 in Serrano-González *et al.*, 1999).

Table 3
Hydrogen-bond geometry (Å, °) for the 295 K data.

$D—H \cdots A$	$D—H$	$H \cdots A$	$D \cdots A$	$D—H \cdots A$
O1A—H1A$\cdots$O1B	0.85	2.56	2.917 (3)	106
O1B—H1BA$\cdots$O1A	0.82	2.27	2.917 (3)	136
O1B—H1BB$\cdots$O1B^i	0.82	2.31	2.912 (3)	131
O1B—H1BC$\cdots$O1B^{ii}	0.85	2.31	2.912 (4)	128
O1C—H1C$\cdots$O1D	0.85	2.27	2.916 (13)	133
O1D—H1DA$\cdots$O1C	0.83	2.26	2.916 (13)	136
O1D—H1DB$\cdots$O1D^{ii}	0.83	2.35	2.947 (13)	130
O1D—H1DC$\cdots$O1D^i	0.84	2.33	2.947 (13)	132

Symmetry codes: (i) $-y + 1, x - y, z$; (ii) $-x + y + 1, -x + 1, z$.

gen bonds (Table 2, entry 1), and is involved in the largest rings, $R_4^3(8)$. All rings are depicted in Fig. 3, along with schematic representations of the corresponding graphs and their pathways [*i.e.* the *constructor graphs* and the *qualitative descriptors*, in the terminology coined by Motherwell *et al.* (1999)].

The tetramer based on *A* and *B* molecules includes 12 hydrogen bonds. Each disordered hydroxy H atom is engaged in a single hydrogen bond, and each O atom serves three times as acceptor (Fig. 4, left). The hydrogen-bonded supramolecular cluster formed in the tetramer is associated with a topological graph embedded in 3-space, *i.e.* $G(4,6) = [R_3^3(6)\text{-}R_4^3(8)R_3^2(6)]$, for which the faces are the $R(n)$ rings described in Fig. 3. In the parlance of graph theory, the finite directed graph $G(4,6)$ based on the '*pyramidal tetramer*' mentioned by Ferguson *et al.* is regular, complete and intrinsically chiral (Flapan, 1995). The four nodes for $G(4,6)$ are provided by four molecules (or four hydroxy O atoms for simplicity) and the six arrows are oriented O—H$\cdots$O hydrogen bonds, the tail of the arrow being the donor OH group and the head being the acceptor O atom. It is noteworthy that for each right-handed $R(n)$ ring, there is one related left-handed ring, as illustrated in Fig. 3. For example, in the first-level $R_3^3(6)$ subgraph embedded in the 2-space, arrows rotate clockwise around the crystallographic threefold axis for the ring including arrows O1B—H1BB$\cdots$O1B (*Rectus* face for topological graph *G*), and anticlockwise for the ring including arrows O1B—H1BC$\cdots$O1B (*Sinister* face for topological graph *G*).

A topologically isomorphous graph $G'(4,6)$ can be built with the minor part of the asymmetric unit, including hydrogen bonds similar to those described for the main tetramer, although the relative positions of the 12 H-atom sites is modified through a small rotation around the C1C—O1C axis (Fig. 4, right). Therefore, the mixture of eight molecules built on the asymmetric unit, as represented in Fig. 2, affords a racemic mixture of supramolecular enantiomorphic tetramers ^{sup}R and ^{sup}S built on 24 hydrogen bonds. Obviously, the molecules themselves are achiral, but the supramolecular chirality results from the asymmetric configuration of the hydrogen bonds (Sasaki *et al.*, 2014). Neither the unit cell nor the crystal are chiral objects, since the molecule crystallizes in a centrosymmetric space group, $R\overline{3}$.

The set of 24 hydrogen bonds depicted in Fig. 4 comprises only weak hydrogen bonds, with H$\cdots$O separations in the

range 2.21–2.38 Å and O—H$\cdots$O angles far from linearity, in the range 121.4–138.2°, at 153 K. The refinement using room-temperature data indicates that the supramolecular chiral clusters are retained, although hydrogen bonds are slightly weakened by *ca* 0.06 Å for H$\cdots$O separations (compare Tables 2 and 3). These geometric parameters were compared with those found in other supramolecular networks formed in the crystalline state by tertiary alcohols, using the methodology developed at the CCDC (Wood *et al.*, 2009). Parameters for intermolecular O—H$\cdots$O contacts in tertiary alcohols were retrieved from the current release of the CSD, omitting disordered, polymeric and ionic structures. Hydroxy H-atom positions were normalized within *ConQuest* to O—H = 0.993 Å, in order to avoid systematic errors in contact distances (Bruno *et al.*, 2002). The search was limited to organic compounds not flagged with errors, and reported with $R_1 < 0.075$, affording 1215 hits, corresponding to 1812 raw data (d, θ), where d is the H$\cdots$O distance and θ is the O—H$\cdots$O angle. Only contacts with d shorter than the van der Waals (vdW) distance were retained [$r_{vdW}(H) + r_{vdW}(O) = 2.72$ Å; Bondi, 1964]. Data were converted into spherical polar coordinates (x, y), where $x = (d/2.72)^3$ and $y = 1 - \cos (180 - \theta)$,
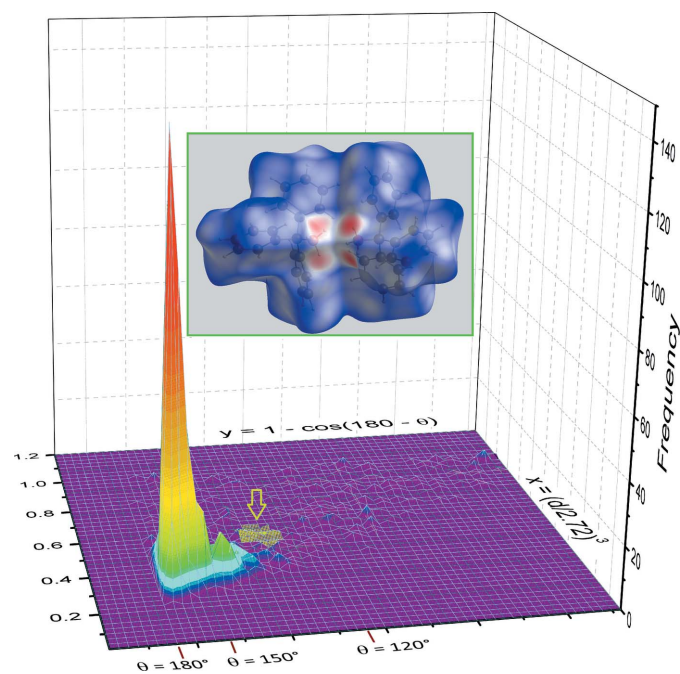
Figure 5
Histogram of the O—H$\cdots$O intermolecular hydrogen-bond geometry in the crystal structures of tertiary alcohols, in spherical polar coordinates (x, y), with the CSD frequency shown in the third dimension (OriginLab, 2012). A $\log_{10}$ rainbow colour scheme is used to highlight small frequencies. Some values for the O—H$\cdots$O angles θ are reported on axis *y*, for reference. Note the similarity of the distribution with that depicted in the CCDC article about the directionality of hydrogen bonds (Wood *et al.*, 2009; see Fig. 2 in this article). The green patch marked with an arrow in the (x, y) plane defines the area for hydrogen bonds in the *A*/*B* tetrameric cluster of the title compound at 153 K. The inset shows the Hirshfeld surface mapped over d (-1 to 1 Å) for the *A*/*B* molecules at 153 K (Turner *et al.*, 2017); each of the four red patches on the surface is related to a single node for the topological graph $G(4,6)$ of the *A*/*B* tetramer (see Fig. 3).

Table 4
Comparison between the three X-ray structures of triphenylmethanol determined at room temperature.

	1992[a]	1999[b]	2019[c]
Date of publication			
Diffractometer	CAD-4	R-Axis II	Stadivari
Detector	NaI scintillator	Image plate	HPAD[d]
T (K)	294	293	295
No. independent reflections	2467	3448	4523
Refined parameters	253	322	483
Data resolution (Å)	0.89	0.82	0.77
Range for σ(C—C)	0.040–0.007 Å	–	0.020–0.003 Å

Notes and references: (a) Ferguson et al. (1992); (b) Serrano-González et al. (1999); (c) this work; (d) Hybrid Pixel Array Detector.

assuming that d and θ are expressed in Å and °, respectively (Lommerse et al., 1996). A two-dimensional (2D) frequency binning histogram representation of the (x, y) distribution shows a sharp peak about $(d, \theta) = (1.82$ Å, $180°)$, as expected for O—H···O hydrogen bonds (Fig. 5). A significant frequency is still observed about $(d, \theta) = (1.87$ Å, $145°)$. Outside these well-defined territories, the observed frequency collapses.

Interestingly, the title compound displays O—H···O contacts on the borderline between truly hydrogen-bonded alcohols and the near-zero frequency area (see green patch on the ground level in Fig. 5). However, although of very limited strength, hydrogen bonds in the tetramers depicted in Fig. 3 are genuinely present, as reflected in the Hirshfeld surface for any pair of molecules involved in a tetrameric supramolecular cluster (Fig. 5, inset). In other words, triphenylmethanol could represent the boundary between hydrogen-bonded and non-hydrogen-bonded tertiary alcohols. This also opens the possibility that a phase transition occurs for triphenylmethanol somewhere between $T = 293$ and 433 K (melting point), if thermal energy kT is able to dismantle the network of weak hydrogen bonds.

In order to evaluate the stability of the noncovalent bonds in this crystal, George Ferguson and co-workers came across a more chemical strategy, by determining the crystal structures of molecules isoelectronic with triphenylmethanol (Glidewell & Ferguson, 1994). Their hypothesis was that 'with only modest changes in the steric demands at the unique central C atom, while keeping the number of hydrogen-bond donors and acceptors unchanged, the patterns of hydrogen bonding can be altered drastically'. Indeed, diphenyl(pyridin-4-yl)methanol has a simple achiral supramolecular structure based on $C(7)$ chains. For triphenylmethanamine, two polymorphic forms have been described: the orthorhombic phase does not form hydrogen bonds at all (Glidewell & Ferguson, 1994), while the triclinic phase features dimers through the formation of N—H···N hydrogen bonds, due to the statistical disordering of the amino H atoms (Khrustalev et al., 2009; Schulz et al., 2013). The NH$_2$ group then displays a geometry reminiscent of that of the OH groups in triphenylmethanol. However, no chiral supramolecular clusters are formed with the amine, and the asymmetric unit includes a single nondisordered molecule. A rhombohedral polymorph for this amine has also been deposited recently; unfortunately, after inspection of this

structure, it turns out that the formula is wrong: the diffracted crystal was almost certainly triphenylmethanol (Bagchi et al., 2014; $R\overline{3}$ space group, $T = 298$ K, $R_1 = 10\%$). In the opposite direction, strong O—H···O hydrogen bonds can be restored in sterically hindered tertiary alcohols by just adding a methylene group: in the crystal structure of triphenylethanol, Ph$_3$CCH$_2$OH (nondisordered $P2_1/c$ crystal, $Z' = 2$; Ferguson et al., 1994), molecules aggregate into discrete achiral $R_4^4(8)$ rings. In comparison with triphenylmethanol, the prochiral character of the supramolecular structure is lost, and the compound lies within a sharp peak of 'normal' crystal structures in a (x, y) distribution similar to that depicted for tertiary alcohols in Fig. 5.

4. Concluding remarks

Triphenylmethanol is a small simple molecule with a structure unexpectedly difficult to refine compared, for example, to that of triphenylsilanol (Bowes et al., 2002). It is worthwhile to consider the evolution of X-ray diffractometry over the last 25 years, using triphenylmethanol as a benchmark (Table 4; data at room temperature were retained in order to avoid biases). The time taken for data collection is almost identical in the three cases, ca 20–30 h, and there is little doubt that the diffracted samples were of similar quality. Over time, a steady progress is noted. Development of new technologies for the detection of scattered X-ray photons seems to be the key point, in such a way that location of tiny fractions of electrons in the crystal space is now routinely affordable, outside the multipole density formalism. There is indeed a consensus that the hybrid pixel detectors with CdTe or GaAs sensors represent the ultimate state-of-art technology in this field, since they detect all scattered X-rays, with 100% efficiency and without any noise (Allé et al., 2016). For the herein presented study, a Pilatus detector was used, with a 1000 µm-thick silicon sensor, which has a quantum efficiency of 50% for 22.2 keV photons (Ag $K\alpha$ radiation).

References

Aliev, A. E., MacLean, E. J., Harris, K. D. M., Kariuki, B. M. & Glidewell, C. (1998). J. Phys. Chem. B, **102**, 2165–2175.
Allé, P., Wenger, E., Dahaoui, S., Schaniel, D. & Lecomte, C. (2016). Phys. Scr. **91**, 063001.
Bagchi, V., Paraskevopoulou, P., Das, P., Chi, L., Wang, Q., Choudhury, A., Mathieson, J. S., Cronin, L., Pardue, D. B., Cundari, T. R., Mitrikas, G., Sanakis, Y. & Stavropoulos, P. (2014). J. Am. Chem. Soc. **136**, 11362–11381.

Barton, D. H. R., Magnus, P. D., Smith, G., Streckert, G. & Zurr, D. (1972). *J. Chem. Soc. Perkin Trans. 1*, pp. 542–552.

Batisai, E., Su, H. & Nassimbeni, L. R. (2016). *CrystEngComm*, **18**, 5952–5958.

Batsanov, A. S. (2018). *Acta Cryst.* E**74**, 570–574.

Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.

Bowes, K. F., Glidewell, C. & Low, J. N. (2002). *Acta Cryst.* C**58**, o409–o415.

Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.

Dobrzycki, L. (2018). *Z. Kristallogr. Cryst. Mater.* **233**, 41–49.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Eckardt, K., Paulus, H., Fuess, H., Onoda-Yamamuro, N., Ikeda, R. & Weiss, A. (1999). *J. Inclusion Phenom. Macrocycl. Chem.* **35**, 431–449.

Ferguson, G., Gallagher, J. F., Glidewell, C., Low, J. N. & Scrimgeour, S. N. (1992). *Acta Cryst.* C**48**, 1272–1275.

Ferguson, G., Glidewell, C. & Zakaria, C. M. (1994). *Acta Cryst.* C**50**, 928–931.

Flapan, E. (1995). *J. Mol. Struct. (Theochem)*, **336**, 157–164.

Glidewell, C. & Ferguson, G. (1994). *Acta Cryst.* C**50**, 924–928.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Khrustalev, V. N., Borisova, I. V., Zemlyansky, N. N. & Antipin, M. Y. (2009). *Acta Cryst.* C**65**, o31–o34.

Lommerse, J. P. M., Stone, A. J., Taylor, R. & Allen, F. H. (1996). *J. Am. Chem. Soc.* **118**, 3108–3116.

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.

Majerz, I. & Natkaniec, I. (2006). *J. Mol. Struct.* **788**, 93–101.

Malarski, Z. (1974). *Mol. Cryst. Liq. Cryst.* **25**, 259–272.

Mootz, D. & Stäben, D. (1993). *Z. Naturforsch. Teil B*, **48**, 1325–1330.

Motherwell, W. D. S., Shields, G. P. & Allen, F. H. (1999). *Acta Cryst.* B**55**, 1044–1056.

OriginLab (2012). *OriginPro 9.1*. OriginLab Corporation, Northampton, MA, USA.

Sasaki, T., Ida, Y., Isaki, I., Yuge, T., Uchida, Y., Tohnai, N. & Miyata, M. (2014). *Chem. Eur. J.* **20**, 2478–2487.

Schröder, L., Watkin, D. J., Cousson, A., Cooper, R. I. & Paulus, W. (2004). *J. Appl. Cryst.* **37**, 545–550.

Schulz, A., Villinger, A. & Westenkirchner, A. (2013). *Inorg. Chem.* **52**, 11457–11468.

Serrano-González, H., Harris, K. D. M., Wilson, C. C., Aliev, A. E., Kitchin, S. J., Kariuki, B. M., Bach-Vergés, M., Glidewell, C., MacLean, E. J. & Kagunya, W. W. (1999). *J. Phys. Chem. B*, **103**, 6215–6223.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015a). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015b). *Acta Cryst.* C**71**, 3–8.

Steiner, T. (2000). *Acta Cryst.* C**56**, 1033–1034.

Stoe & Cie (2018). *X-AREA* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.

Thorn, A., Dittrich, B. & Sheldrick, G. M. (2012). *Acta Cryst.* A**68**, 448–451.

Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *CrystalExplorer17*. University of Western Australia.

Weber, E., Skobridis, K. & Goldberg, I. (1989). *J. Chem. Soc. Chem. Commun.* pp. 1195–1197.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

Wood, P. A., Allen, F. H. & Pidcock, E. (2009). *CrystEngComm*, **11**, 1563–1571.

Zeiss, H. H. & Tsutsui, M. (1953). *J. Am. Chem. Soc.* **75**, 897–900.

supporting information

Deciphering the hydrogen-bonding scheme in the crystal structure of triphenyl-methanol: a tribute to George Ferguson and co-workers

Tomasa Rodríguez Tzompantzi, Aldo Guillermo Amaro Hernández, Rosa Luisa Meza-León and Sylvain Bernès

Computing details

For both structures, data collection: *X-AREA* (Stoe & Cie, 2018); cell refinement: *X-AREA* (Stoe & Cie, 2018); data reduction: *X-AREA* (Stoe & Cie, 2018); program(s) used to solve structure: SHELXT2018 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Triphenylmethanol (153K_data)

Crystal data

$C_{19}H_{16}O$	Melting point: 433 K
$M_r = 260.32$	Ag $K\alpha$ radiation, $\lambda = 0.56083$ Å
Trigonal, $R\bar{3}:H$	Cell parameters from 38242 reflections
$a = 19.1399$ (5) Å	$\theta = 2.3–27.9°$
$c = 26.7399$ (9) Å	$\mu = 0.05$ mm^{-1}
$V = 8483.4$ (5) Å^3	$T = 153$ K
$Z = 24$	Prism, colourless
$F(000) = 3312$	$0.33 \times 0.29 \times 0.25$ mm
$D_x = 1.223$ Mg m^{-3}	

Data collection

Stoe Stadivari diffractometer	$T_{min} = 0.419$, $T_{max} = 1.000$
Radiation source: Sealed X-ray tube, Axo Astix-f Microfocus source	99452 measured reflections
	4399 independent reflections
Graded multilayer mirror monochromator	2222 reflections with $I > 2\sigma(I)$
Detector resolution: 5.81 pixels mm^{-1}	$R_{int} = 0.069$
ω scans	$\theta_{max} = 21.5°$, $\theta_{min} = 2.3°$
Absorption correction: multi-scan (X-AREA; Stoe & Cie, 2018)	$h = -24\rightarrow24$
	$k = -24\rightarrow24$
	$l = -34\rightarrow34$

Refinement

Refinement on F^2	483 parameters
Least-squares matrix: full	72 restraints
$R[F^2 > 2\sigma(F^2)] = 0.052$	0 constraints
$wR(F^2) = 0.167$	Primary atom site location: dual
$S = 1.00$	Secondary atom site location: difference Fourier map
4399 reflections	

Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 2.9871P]$
  where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1A	0.666667	0.333333	0.51277 (9)	0.0911 (10)	0.7436 (17)
H1A	0.708695	0.373627	0.525137	0.137*	0.2479 (6)
C1A	0.666667	0.333333	0.45915 (12)	0.0585 (9)	0.7436 (17)
C2A	0.58184 (15)	0.30928 (15)	0.44155 (8)	0.0574 (5)	0.7436 (17)
C3A	0.53537 (17)	0.33357 (18)	0.46817 (10)	0.0780 (7)	0.7436 (17)
H3A	0.555863	0.362570	0.498506	0.094*	0.7436 (17)
C4A	0.4606 (4)	0.3168 (5)	0.4518 (3)	0.096 (2)	0.7436 (17)
H4A	0.429793	0.333886	0.470662	0.115*	0.7436 (17)
C5A	0.4305 (4)	0.2749 (5)	0.4078 (3)	0.094 (3)	0.7436 (17)
H5A	0.379487	0.264579	0.395771	0.113*	0.7436 (17)
C6A	0.4737 (4)	0.2481 (5)	0.3813 (3)	0.086 (2)	0.7436 (17)
H6A	0.452087	0.217872	0.351492	0.103*	0.7436 (17)
C7A	0.5487 (4)	0.2652 (4)	0.3981 (2)	0.0698 (15)	0.7436 (17)
H7A	0.578423	0.246450	0.379498	0.084*	0.7436 (17)
O1B	0.76424 (10)	0.36344 (13)	0.60040 (7)	0.1001 (7)	0.7436 (17)
H1BA	0.761666	0.351068	0.570135	0.150*	0.2479 (6)
H1BB	0.749287	0.395976	0.605330	0.150*	0.2479 (6)
H1BC	0.730448	0.319412	0.615019	0.150*	0.2479 (6)
C1B	0.84281 (12)	0.38633 (15)	0.61999 (8)	0.0648 (6)	0.7436 (17)
C2B	0.86638 (13)	0.32631 (14)	0.59957 (8)	0.0657 (6)	0.7436 (17)
C3B	0.8535 (2)	0.3054 (2)	0.54985 (11)	0.1044 (11)	0.7436 (17)
H3B	0.830275	0.328339	0.528779	0.125*	0.7436 (17)
C4B	0.8740 (5)	0.2516 (6)	0.5304 (3)	0.119 (3)	0.7436 (17)
H4B	0.863199	0.236550	0.496240	0.143*	0.7436 (17)
C5B	0.9095 (5)	0.2196 (5)	0.5591 (3)	0.109 (3)	0.7436 (17)
H5B	0.924530	0.183335	0.545252	0.131*	0.7436 (17)
C6B	0.9231 (4)	0.2407 (4)	0.6084 (3)	0.093 (2)	0.7436 (17)
H6B	0.947373	0.218561	0.629241	0.112*	0.7436 (17)
C7B	0.9018 (2)	0.2941 (2)	0.62816 (16)	0.0777 (9)	0.7436 (17)
H7B	0.912098	0.308569	0.662466	0.093*	0.7436 (17)
C8B	0.90166 (14)	0.47184 (15)	0.60289 (9)	0.0668 (6)	0.7436 (17)
C9B	0.8772 (2)	0.5287 (2)	0.59841 (10)	0.0883 (9)	0.7436 (17)
H9B	0.822728	0.513460	0.605400	0.106*	0.7436 (17)
C10B	0.9281 (6)	0.6036 (5)	0.5846 (3)	0.111 (3)	0.7436 (17)
H10B	0.908782	0.640297	0.580162	0.133*	0.7436 (17)
C11B	1.0077 (5)	0.6296 (4)	0.5767 (3)	0.130 (3)	0.7436 (17)
H11B	1.043803	0.684533	0.568696	0.156*	0.7436 (17)
C12B	1.0361 (5)	0.5760 (6)	0.5802 (4)	0.121 (3)	0.7436 (17)
H12B	1.091060	0.592640	0.573739	0.145*	0.7436 (17)
C13B	0.9815 (3)	0.4974 (3)	0.59348 (16)	0.0874 (11)	0.7436 (17)

H13B	0.999752	0.459704	0.596214	0.105*	0.7436 (17)
C14B	0.83584 (19)	0.38110 (17)	0.67725 (10)	0.0612 (6)	0.7436 (17)
C15B	0.77028 (16)	0.3162 (2)	0.69875 (11)	0.0917 (9)	0.7436 (17)
H15B	0.728841	0.277251	0.677965	0.110*	0.7436 (17)
C16B	0.7637 (3)	0.3068 (4)	0.7494 (2)	0.0951 (17)	0.7436 (17)
H16B	0.717770	0.261153	0.763094	0.114*	0.7436 (17)
C17B	0.8224 (3)	0.3621 (3)	0.78128 (17)	0.0783 (11)	0.7436 (17)
H17B	0.818095	0.355011	0.816530	0.094*	0.7436 (17)
C18B	0.88692 (19)	0.42746 (19)	0.75964 (10)	0.0742 (8)	0.7436 (17)
H18B	0.928135	0.466765	0.780380	0.089*	0.7436 (17)
C19B	0.8933 (3)	0.4374 (4)	0.7088 (2)	0.0655 (12)	0.7436 (17)
H19B	0.938180	0.483932	0.694994	0.079*	0.7436 (17)
O1C	0.666667	0.333333	0.6432 (3)	0.083 (3)	0.2564 (17)
H1C	0.682226	0.379070	0.629806	0.124*	0.0855 (6)
C1C	0.666667	0.333333	0.6960 (4)	0.058 (3)	0.2564 (17)
C2C	0.7503 (5)	0.3564 (5)	0.7147 (3)	0.073 (2)	0.2564 (17)
C3C	0.7666 (11)	0.3251 (10)	0.7590 (5)	0.113 (8)	0.2564 (17)
H3C	0.724063	0.289629	0.780547	0.136*	0.2564 (17)
C4C	0.8465 (10)	0.3481 (10)	0.7697 (5)	0.117 (5)	0.2564 (17)
H4C	0.858261	0.325808	0.798051	0.140*	0.2564 (17)
C5C	0.9068 (7)	0.4009 (8)	0.7409 (7)	0.149 (7)	0.2564 (17)
H5C	0.960816	0.418783	0.750763	0.179*	0.2564 (17)
C6C	0.8931 (12)	0.4299 (17)	0.6977 (9)	0.124 (10)	0.2564 (17)
H6C	0.936377	0.464379	0.676274	0.149*	0.2564 (17)
C7C	0.8166 (5)	0.4083 (6)	0.6862 (4)	0.094 (3)	0.2564 (17)
H7C	0.807355	0.430151	0.656715	0.113*	0.2564 (17)
O1D	0.7440 (3)	0.4306 (3)	0.55748 (19)	0.0885 (17)	0.2564 (17)
H1DA	0.730812	0.432220	0.587335	0.133*	0.0855 (6)
H1DB	0.761560	0.399257	0.554882	0.133*	0.0855 (6)
H1DC	0.701323	0.413280	0.540448	0.133*	0.0855 (6)
C1D	0.8005 (4)	0.5111 (4)	0.5411 (2)	0.0642 (17)	0.2564 (17)
C2D	0.7764 (3)	0.5690 (4)	0.5642 (2)	0.0642 (18)	0.2564 (17)
C3D	0.7632 (5)	0.5676 (6)	0.6149 (3)	0.106 (3)	0.2564 (17)
H3D	0.766173	0.527914	0.634760	0.128*	0.2564 (17)
C4D	0.7462 (7)	0.6211 (9)	0.6377 (5)	0.106 (5)	0.2564 (17)
H4D	0.738431	0.618454	0.672879	0.127*	0.2564 (17)
C5D	0.7400 (14)	0.6797 (14)	0.6101 (8)	0.108 (8)	0.2564 (17)
H5D	0.729664	0.718341	0.625539	0.129*	0.2564 (17)
C6D	0.7497 (13)	0.6782 (14)	0.5595 (8)	0.105 (7)	0.2564 (17)
H6D	0.746374	0.717334	0.539303	0.126*	0.2564 (17)
C7D	0.7639 (18)	0.6222 (16)	0.5368 (8)	0.111 (8)	0.2564 (17)
H7D	0.765172	0.620367	0.501360	0.134*	0.2564 (17)
C8D	0.8844 (4)	0.5289 (4)	0.5587 (3)	0.0620 (17)	0.2564 (17)
C9D	0.9455 (10)	0.6073 (9)	0.5784 (6)	0.089 (6)	0.2564 (17)
H9D	0.932585	0.648849	0.582298	0.107*	0.2564 (17)
C10D	1.0181 (9)	0.6216 (10)	0.5909 (5)	0.095 (7)	0.2564 (17)
H10D	1.058560	0.673426	0.601934	0.113*	0.2564 (17)
C11D	1.0330 (11)	0.5589 (12)	0.5873 (8)	0.096 (8)	0.2564 (17)

H11D	1.082620	0.566820	0.600425	0.115*	0.2564 (17)
C12D	0.9796 (8)	0.4827 (8)	0.5654 (5)	0.101 (4)	0.2564 (17)
H12D	0.994971	0.443504	0.558556	0.121*	0.2564 (17)
C13D	0.9044 (5)	0.4705 (4)	0.5552 (4)	0.098 (3)	0.2564 (17)
H13D	0.863835	0.418145	0.544928	0.118*	0.2564 (17)
C14D	0.7983 (4)	0.5139 (4)	0.4833 (3)	0.0577 (15)	0.2564 (17)
C15D	0.7290 (4)	0.4634 (4)	0.4585 (3)	0.0679 (18)	0.2564 (17)
H15D	0.682472	0.426339	0.476747	0.081*	0.2564 (17)
C16D	0.7256 (13)	0.4656 (13)	0.4069 (6)	0.084 (7)	0.2564 (17)
H16D	0.677505	0.428401	0.390046	0.101*	0.2564 (17)
C17D	0.7909 (12)	0.5208 (14)	0.3795 (6)	0.068 (5)	0.2564 (17)
H17D	0.787198	0.524908	0.344309	0.082*	0.2564 (17)
C18D	0.8615 (12)	0.5698 (12)	0.4044 (6)	0.073 (4)	0.2564 (17)
H18D	0.908149	0.606844	0.386238	0.087*	0.2564 (17)
C19D	0.8650 (11)	0.5653 (11)	0.4560 (6)	0.085 (5)	0.2564 (17)
H19D	0.914603	0.598511	0.472742	0.102*	0.2564 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.1199 (16)	0.1199 (16)	0.0335 (13)	0.0599 (8)	0.000	0.000
C1A	0.0713 (15)	0.0713 (15)	0.0329 (16)	0.0357 (7)	0.000	0.000
C2A	0.0639 (14)	0.0594 (14)	0.0467 (12)	0.0293 (12)	0.0094 (11)	0.0053 (10)
C3A	0.0717 (18)	0.0823 (19)	0.0780 (17)	0.0371 (16)	0.0175 (14)	−0.0053 (14)
C4A	0.075 (4)	0.092 (4)	0.124 (4)	0.044 (3)	0.027 (3)	0.002 (3)
C5A	0.046 (2)	0.088 (5)	0.133 (5)	0.022 (2)	0.002 (2)	0.016 (3)
C6A	0.064 (3)	0.088 (5)	0.095 (3)	0.029 (3)	−0.013 (2)	−0.001 (3)
C7A	0.072 (3)	0.087 (3)	0.0562 (17)	0.044 (2)	−0.005 (2)	−0.0042 (17)
O1B	0.0517 (10)	0.1542 (19)	0.0920 (13)	0.0496 (11)	−0.0238 (9)	−0.0112 (12)
C1B	0.0431 (11)	0.0886 (16)	0.0611 (13)	0.0318 (11)	−0.0094 (9)	−0.0070 (11)
C2B	0.0477 (12)	0.0767 (15)	0.0608 (13)	0.0221 (11)	−0.0055 (10)	−0.0089 (11)
C3B	0.129 (3)	0.127 (3)	0.0727 (18)	0.075 (2)	−0.0188 (17)	−0.0283 (18)
C4B	0.164 (7)	0.138 (6)	0.079 (3)	0.093 (5)	−0.013 (4)	−0.039 (4)
C5B	0.126 (6)	0.102 (5)	0.104 (4)	0.062 (4)	0.017 (3)	−0.026 (3)
C6B	0.103 (4)	0.100 (5)	0.096 (4)	0.066 (4)	0.002 (3)	−0.008 (3)
C7B	0.081 (2)	0.086 (3)	0.0704 (19)	0.045 (2)	−0.0051 (18)	−0.0155 (19)
C8B	0.0611 (14)	0.0884 (17)	0.0549 (13)	0.0403 (13)	−0.0037 (10)	−0.0008 (12)
C9B	0.106 (2)	0.126 (3)	0.0599 (17)	0.078 (2)	0.0093 (15)	0.0162 (16)
C10B	0.145 (7)	0.133 (6)	0.081 (3)	0.090 (5)	0.025 (3)	0.037 (3)
C11B	0.157 (7)	0.094 (4)	0.105 (5)	0.036 (5)	0.020 (4)	0.027 (3)
C12B	0.086 (5)	0.100 (4)	0.138 (7)	0.017 (3)	0.024 (4)	0.026 (4)
C13B	0.063 (2)	0.082 (3)	0.113 (3)	0.0326 (18)	0.006 (2)	0.006 (2)
C14B	0.0430 (14)	0.0768 (19)	0.0647 (14)	0.0307 (14)	−0.0015 (12)	−0.0041 (12)
C15B	0.0624 (16)	0.099 (2)	0.0743 (18)	0.0114 (15)	0.0047 (13)	−0.0138 (15)
C16B	0.072 (3)	0.098 (3)	0.078 (2)	0.015 (2)	0.0179 (18)	−0.004 (2)
C17B	0.087 (3)	0.093 (3)	0.0624 (17)	0.050 (2)	0.0047 (17)	−0.0068 (16)
C18B	0.0747 (19)	0.078 (2)	0.0666 (16)	0.0360 (16)	−0.0144 (13)	−0.0065 (14)
C19B	0.055 (2)	0.075 (3)	0.0624 (18)	0.029 (2)	−0.0078 (15)	−0.0024 (17)

O1C	0.105 (4)	0.105 (4)	0.039 (4)	0.052 (2)	0.000	0.000
C1C	0.066 (4)	0.066 (4)	0.041 (5)	0.033 (2)	0.000	0.000
C2C	0.095 (6)	0.080 (5)	0.059 (4)	0.054 (5)	0.001 (4)	0.007 (4)
C3C	0.146 (15)	0.121 (14)	0.081 (10)	0.074 (12)	−0.016 (9)	0.034 (10)
C4C	0.140 (15)	0.119 (11)	0.108 (11)	0.077 (11)	−0.046 (10)	0.011 (9)
C5C	0.081 (8)	0.083 (8)	0.28 (2)	0.040 (7)	−0.022 (11)	0.012 (11)
C6C	0.115 (16)	0.126 (18)	0.15 (2)	0.074 (15)	0.021 (14)	0.042 (16)
C7C	0.072 (6)	0.108 (8)	0.121 (8)	0.059 (6)	0.024 (5)	0.041 (6)
O1D	0.073 (3)	0.061 (3)	0.097 (4)	0.008 (2)	−0.007 (3)	0.031 (3)
C1D	0.054 (4)	0.047 (3)	0.073 (4)	0.012 (3)	−0.001 (3)	0.017 (3)
C2D	0.041 (3)	0.067 (4)	0.070 (4)	0.015 (3)	0.008 (3)	0.020 (3)
C3D	0.124 (8)	0.133 (8)	0.082 (5)	0.078 (6)	0.051 (5)	0.046 (5)
C4D	0.101 (10)	0.162 (13)	0.087 (8)	0.091 (10)	0.026 (7)	0.014 (8)
C5D	0.082 (10)	0.19 (2)	0.087 (11)	0.091 (12)	−0.019 (7)	−0.024 (11)
C6D	0.124 (18)	0.110 (14)	0.097 (12)	0.072 (13)	−0.006 (11)	0.011 (10)
C7D	0.126 (13)	0.149 (19)	0.101 (12)	0.100 (14)	−0.003 (9)	−0.020 (11)
C8D	0.055 (4)	0.059 (4)	0.065 (4)	0.023 (3)	0.006 (3)	0.011 (3)
C9D	0.044 (5)	0.063 (7)	0.133 (15)	0.005 (5)	0.001 (7)	0.025 (7)
C10D	0.060 (6)	0.162 (17)	0.056 (6)	0.052 (8)	−0.010 (5)	−0.050 (8)
C11D	0.072 (13)	0.17 (3)	0.057 (6)	0.071 (17)	0.001 (7)	0.005 (10)
C12D	0.111 (9)	0.101 (8)	0.115 (9)	0.071 (7)	−0.034 (8)	−0.014 (7)
C13D	0.080 (6)	0.057 (4)	0.152 (9)	0.030 (4)	−0.026 (5)	−0.001 (5)
C14D	0.052 (4)	0.040 (3)	0.083 (4)	0.024 (3)	−0.003 (3)	−0.001 (3)
C15D	0.058 (4)	0.053 (4)	0.084 (5)	0.021 (3)	0.000 (4)	−0.002 (4)
C16D	0.071 (8)	0.077 (9)	0.114 (14)	0.044 (7)	−0.033 (8)	−0.027 (8)
C17D	0.093 (11)	0.084 (9)	0.055 (5)	0.065 (9)	−0.006 (5)	−0.010 (5)
C18D	0.072 (7)	0.097 (9)	0.068 (7)	0.056 (7)	0.004 (5)	0.007 (6)
C19D	0.075 (8)	0.084 (12)	0.082 (9)	0.029 (7)	−0.002 (6)	0.027 (8)

Geometric parameters (Å, º)

O1A—C1A	1.434 (4)	O1C—C1C	1.411 (11)
O1A—H1A	0.8549	O1C—H1C	0.8500
O1A—H1A^i	0.8549	O1C—H1C^i	0.8500
O1A—H1A^{ii}	0.8549	O1C—H1C^{ii}	0.8501
C1A—C2A	1.524 (3)	C1C—C2C	1.517 (8)
C1A—C2A^{ii}	1.524 (3)	C1C—C2C^{ii}	1.518 (8)
C1A—C2A^i	1.524 (3)	C1C—C2C^i	1.518 (8)
C2A—C3A	1.388 (3)	C2C—C7C	1.384 (10)
C2A—C7A	1.389 (6)	C2C—C3C	1.430 (14)
C3A—C4A	1.373 (7)	C3C—C4C	1.394 (17)
C3A—H3A	0.9500	C3C—H3C	0.9500
C4A—C5A	1.377 (9)	C4C—C5C	1.335 (15)
C4A—H4A	0.9500	C4C—H4C	0.9500
C5A—C6A	1.368 (8)	C5C—C6C	1.363 (18)
C5A—H5A	0.9500	C5C—H5C	0.9500
C6A—C7A	1.379 (7)	C6C—C7C	1.343 (17)
C6A—H6A	0.9500	C6C—H6C	0.9500

C7A—H7A	0.9500	C7C—H7C	0.9500
O1B—C1B	1.438 (2)	O1D—C1D	1.438 (7)
O1B—H1BA	0.8376	O1D—H1DA	0.8426
O1B—H1BB	0.8158	O1D—H1DB	0.8241
O1B—H1BC	0.8580	O1D—H1DC	0.8453
C1B—C8B	1.521 (3)	C1D—C2D	1.527 (9)
C1B—C2B	1.530 (3)	C1D—C8D	1.540 (9)
C1B—C14B	1.536 (3)	C1D—C14D	1.548 (9)
C2B—C7B	1.357 (5)	C2D—C7D	1.368 (16)
C2B—C3B	1.374 (3)	C2D—C3D	1.379 (9)
C3B—C4B	1.375 (8)	C3D—C4D	1.364 (13)
C3B—H3B	0.9500	C3D—H3D	0.9500
C4B—C5B	1.357 (11)	C4D—C5D	1.40 (2)
C4B—H4B	0.9500	C4D—H4D	0.9500
C5B—C6B	1.364 (6)	C5D—C6D	1.368 (15)
C5B—H5B	0.9500	C5D—H5D	0.9500
C6B—C7B	1.381 (7)	C6D—C7D	1.37 (2)
C6B—H6B	0.9500	C6D—H6D	0.9500
C7B—H7B	0.9500	C7D—H7D	0.9500
C8B—C13B	1.374 (5)	C8D—C13D	1.354 (9)
C8B—C9B	1.389 (4)	C8D—C9D	1.463 (15)
C9B—C10B	1.320 (8)	C9D—C10D	1.318 (17)
C9B—H9B	0.9500	C9D—H9D	0.9500
C10B—C11B	1.364 (9)	C10D—C11D	1.37 (2)
C10B—H10B	0.9500	C10D—H10D	0.9500
C11B—C12B	1.382 (11)	C11D—C12D	1.423 (18)
C11B—H11B	0.9500	C11D—H11D	0.9500
C12B—C13B	1.382 (10)	C12D—C13D	1.367 (12)
C12B—H12B	0.9500	C12D—H12D	0.9500
C13B—H13B	0.9500	C13D—H13D	0.9500
C14B—C15B	1.374 (4)	C14D—C15D	1.361 (9)
C14B—C19B	1.376 (7)	C14D—C19D	1.369 (16)
C15B—C16B	1.363 (6)	C15D—C16D	1.383 (16)
C15B—H15B	0.9500	C15D—H15D	0.9500
C16B—C17B	1.386 (7)	C16D—C17D	1.376 (18)
C16B—H16B	0.9500	C16D—H16D	0.9500
C17B—C18B	1.371 (5)	C17D—C18D	1.371 (18)
C17B—H17B	0.9500	C17D—H17D	0.9500
C18B—C19B	1.370 (7)	C18D—C19D	1.386 (17)
C18B—H18B	0.9500	C18D—H18D	0.9500
C19B—H19B	0.9500	C19D—H19D	0.9500
C1A—O1A—H1A	112.8	C14B—C19B—H19B	119.4
C1A—O1A—H1A^{i}	112.8	C1C—O1C—H1C	114.9
C1A—O1A—H1A^{ii}	112.754 (1)	C1C—O1C—H1C^{i}	114.914 (3)
H1A—O1A—H1A^{i}	106.0	H1C—O1C—H1C^{i}	103.5
H1A—O1A—H1A^{ii}	106.0	O1C—C1C—C2C	109.3 (4)
H1A^{i}—O1A—H1A^{ii}	106.0	O1C—C1C—C2C^{ii}	109.3 (4)

O1A—C1A—C2A	107.99 (14)	C2C—C1C—C2C^ii	109.6 (4)
O1A—C1A—C2A^ii	107.99 (14)	O1C—C1C—C2C^i	109.3 (4)
C2A—C1A—C2A^ii	110.91 (13)	C2C—C1C—C2C^i	109.6 (4)
O1A—C1A—C2A^i	107.99 (14)	C2C^ii—C1C—C2C^i	109.6 (4)
C2A—C1A—C2A^i	110.91 (13)	C7C—C2C—C3C	116.3 (10)
C2A^ii—C1A—C2A^i	110.90 (13)	C7C—C2C—C1C	118.8 (7)
C3A—C2A—C7A	117.3 (4)	C3C—C2C—C1C	124.8 (10)
C3A—C2A—C1A	120.3 (2)	C4C—C3C—C2C	118.2 (13)
C7A—C2A—C1A	122.4 (4)	C4C—C3C—H3C	120.9
C4A—C3A—C2A	121.7 (4)	C2C—C3C—H3C	120.9
C4A—C3A—H3A	119.1	C5C—C4C—C3C	121.1 (12)
C2A—C3A—H3A	119.1	C5C—C4C—H4C	119.4
C3A—C4A—C5A	119.5 (6)	C3C—C4C—H4C	119.4
C3A—C4A—H4A	120.2	C4C—C5C—C6C	121.9 (13)
C5A—C4A—H4A	120.2	C4C—C5C—H5C	119.0
C6A—C5A—C4A	120.3 (6)	C6C—C5C—H5C	119.0
C6A—C5A—H5A	119.8	C7C—C6C—C5C	118.0 (17)
C4A—C5A—H5A	119.8	C7C—C6C—H6C	121.0
C5A—C6A—C7A	119.7 (7)	C5C—C6C—H6C	121.0
C5A—C6A—H6A	120.1	C6C—C7C—C2C	124.2 (12)
C7A—C6A—H6A	120.1	C6C—C7C—H7C	117.9
C6A—C7A—C2A	121.4 (7)	C2C—C7C—H7C	117.9
C6A—C7A—H7A	119.3	C1D—O1D—H1DA	109.2
C2A—C7A—H7A	119.3	C1D—O1D—H1DB	113.2
C1B—O1B—H1BA	110.1	C1D—O1D—H1DC	108.5
C1B—O1B—H1BB	114.9	H1DA—O1D—H1DB	110.2
C1B—O1B—H1BC	107.0	H1DA—O1D—H1DC	106.0
H1BA—O1B—H1BB	112.2	H1DB—O1D—H1DC	109.5
H1BA—O1B—H1BC	104.7	O1D—C1D—C2D	108.5 (5)
H1BB—O1B—H1BC	107.2	O1D—C1D—C8D	106.6 (5)
O1B—C1B—C8B	108.49 (19)	C2D—C1D—C8D	112.1 (5)
O1B—C1B—C2B	107.29 (18)	O1D—C1D—C14D	108.8 (5)
C8B—C1B—C2B	111.28 (18)	C2D—C1D—C14D	110.8 (5)
O1B—C1B—C14B	107.45 (19)	C8D—C1D—C14D	110.0 (5)
C8B—C1B—C14B	111.3 (2)	C7D—C2D—C3D	116.3 (11)
C2B—C1B—C14B	110.8 (2)	C7D—C2D—C1D	123.6 (10)
C7B—C2B—C3B	118.1 (3)	C3D—C2D—C1D	120.1 (6)
C7B—C2B—C1B	122.8 (2)	C4D—C3D—C2D	122.3 (9)
C3B—C2B—C1B	119.1 (2)	C4D—C3D—H3D	118.9
C2B—C3B—C4B	120.4 (5)	C2D—C3D—H3D	118.9
C2B—C3B—H3B	119.8	C3D—C4D—C5D	121.1 (13)
C4B—C3B—H3B	119.8	C3D—C4D—H4D	119.5
C5B—C4B—C3B	121.3 (6)	C5D—C4D—H4D	119.5
C5B—C4B—H4B	119.4	C6D—C5D—C4D	116.0 (18)
C3B—C4B—H4B	119.4	C6D—C5D—H5D	122.0
C4B—C5B—C6B	118.5 (7)	C4D—C5D—H5D	122.0
C4B—C5B—H5B	120.7	C5D—C6D—C7D	122 (2)
C6B—C5B—H5B	120.7	C5D—C6D—H6D	118.8

C5B—C6B—C7B	120.3 (6)	C7D—C6D—H6D	118.8
C5B—C6B—H6B	119.8	C2D—C7D—C6D	121.5 (19)
C7B—C6B—H6B	119.8	C2D—C7D—H7D	119.2
C2B—C7B—C6B	121.3 (4)	C6D—C7D—H7D	119.2
C2B—C7B—H7B	119.3	C13D—C8D—C9D	117.5 (9)
C6B—C7B—H7B	119.3	C13D—C8D—C1D	119.3 (6)
C13B—C8B—C9B	117.1 (3)	C9D—C8D—C1D	123.3 (9)
C13B—C8B—C1B	122.1 (3)	C10D—C9D—C8D	121.6 (16)
C9B—C8B—C1B	120.7 (2)	C10D—C9D—H9D	119.2
C10B—C9B—C8B	121.4 (5)	C8D—C9D—H9D	119.2
C10B—C9B—H9B	119.3	C9D—C10D—C11D	117.4 (16)
C8B—C9B—H9B	119.3	C9D—C10D—H10D	121.3
C9B—C10B—C11B	121.5 (8)	C11D—C10D—H10D	121.3
C9B—C10B—H10B	119.3	C10D—C11D—C12D	124.7 (14)
C11B—C10B—H10B	119.3	C10D—C11D—H11D	117.6
C10B—C11B—C12B	120.1 (8)	C12D—C11D—H11D	117.6
C10B—C11B—H11B	119.9	C13D—C12D—C11D	114.4 (12)
C12B—C11B—H11B	119.9	C13D—C12D—H12D	122.8
C11B—C12B—C13B	117.4 (8)	C11D—C12D—H12D	122.8
C11B—C12B—H12B	121.3	C8D—C13D—C12D	123.6 (8)
C13B—C12B—H12B	121.3	C8D—C13D—H13D	118.2
C8B—C13B—C12B	122.5 (5)	C12D—C13D—H13D	118.2
C8B—C13B—H13B	118.8	C15D—C14D—C19D	118.6 (9)
C12B—C13B—H13B	118.8	C15D—C14D—C1D	119.7 (6)
C15B—C14B—C19B	117.5 (3)	C19D—C14D—C1D	121.7 (9)
C15B—C14B—C1B	119.1 (2)	C14D—C15D—C16D	120.5 (11)
C19B—C14B—C1B	123.4 (3)	C14D—C15D—H15D	119.7
C16B—C15B—C14B	121.1 (3)	C16D—C15D—H15D	119.7
C16B—C15B—H15B	119.4	C17D—C16D—C15D	121.1 (16)
C14B—C15B—H15B	119.4	C17D—C16D—H16D	119.5
C15B—C16B—C17B	121.6 (4)	C15D—C16D—H16D	119.5
C15B—C16B—H16B	119.2	C18D—C17D—C16D	118.2 (16)
C17B—C16B—H16B	119.2	C18D—C17D—H17D	120.9
C18B—C17B—C16B	116.9 (4)	C16D—C17D—H17D	120.9
C18B—C17B—H17B	121.5	C17D—C18D—C19D	120.2 (16)
C16B—C17B—H17B	121.5	C17D—C18D—H18D	119.9
C19B—C18B—C17B	121.5 (4)	C19D—C18D—H18D	119.9
C19B—C18B—H18B	119.3	C14D—C19D—C18D	121.2 (16)
C17B—C18B—H18B	119.3	C14D—C19D—H19D	119.4
C18B—C19B—C14B	121.2 (5)	C18D—C19D—H19D	119.4
C18B—C19B—H19B	119.4		
O1A—C1A—C2A—C3A	35.5 (2)	O1C—C1C—C2C—C7C	31.0 (9)
C2A^{ii}—C1A—C2A—C3A	−82.7 (3)	C2C^{ii}—C1C—C2C—C7C	150.7 (9)
C2A^{i}—C1A—C2A—C3A	153.6 (2)	C2C^{i}—C1C—C2C—C7C	−88.8 (12)
O1A—C1A—C2A—C7A	−146.7 (4)	O1C—C1C—C2C—C3C	−145.6 (9)
C2A^{ii}—C1A—C2A—C7A	95.1 (4)	C2C^{ii}—C1C—C2C—C3C	−25.8 (12)
C2A^{i}—C1A—C2A—C7A	−28.6 (5)	C2C^{i}—C1C—C2C—C3C	94.6 (9)

C7A—C2A—C3A—C4A	−1.6 (6)	C7C—C2C—C3C—C4C	−0.7 (14)
C1A—C2A—C3A—C4A	176.3 (4)	C1C—C2C—C3C—C4C	175.9 (10)
C2A—C3A—C4A—C5A	−0.1 (9)	C2C—C3C—C4C—C5C	3.2 (17)
C3A—C4A—C5A—C6A	1.9 (12)	C3C—C4C—C5C—C6C	−5 (3)
C4A—C5A—C6A—C7A	−1.9 (12)	C4C—C5C—C6C—C7C	5 (4)
C5A—C6A—C7A—C2A	0.0 (10)	C5C—C6C—C7C—C2C	−2 (4)
C3A—C2A—C7A—C6A	1.7 (8)	C3C—C2C—C7C—C6C	0 (2)
C1A—C2A—C7A—C6A	−176.2 (5)	C1C—C2C—C7C—C6C	−176.6 (19)
O1B—C1B—C2B—C7B	−137.2 (3)	O1D—C1D—C2D—C7D	−126.3 (16)
C8B—C1B—C2B—C7B	104.2 (3)	C8D—C1D—C2D—C7D	116.3 (17)
C14B—C1B—C2B—C7B	−20.2 (4)	C14D—C1D—C2D—C7D	−7.0 (17)
O1B—C1B—C2B—C3B	44.6 (3)	O1D—C1D—C2D—C3D	51.4 (8)
C8B—C1B—C2B—C3B	−73.9 (3)	C8D—C1D—C2D—C3D	−66.0 (8)
C14B—C1B—C2B—C3B	161.7 (3)	C14D—C1D—C2D—C3D	170.8 (6)
C7B—C2B—C3B—C4B	1.8 (6)	C7D—C2D—C3D—C4D	−6.0 (17)
C1B—C2B—C3B—C4B	−180.0 (5)	C1D—C2D—C3D—C4D	176.1 (8)
C2B—C3B—C4B—C5B	−2.0 (11)	C2D—C3D—C4D—C5D	1.0 (17)
C3B—C4B—C5B—C6B	1.3 (13)	C3D—C4D—C5D—C6D	2 (3)
C4B—C5B—C6B—C7B	−0.6 (12)	C4D—C5D—C6D—C7D	1 (4)
C3B—C2B—C7B—C6B	−1.2 (6)	C3D—C2D—C7D—C6D	8 (3)
C1B—C2B—C7B—C6B	−179.3 (4)	C1D—C2D—C7D—C6D	−173.9 (18)
C5B—C6B—C7B—C2B	0.6 (9)	C5D—C6D—C7D—C2D	−6 (4)
O1B—C1B—C8B—C13B	−147.8 (3)	O1D—C1D—C8D—C13D	40.9 (9)
C2B—C1B—C8B—C13B	−30.0 (3)	C2D—C1D—C8D—C13D	159.4 (7)
C14B—C1B—C8B—C13B	94.2 (3)	C14D—C1D—C8D—C13D	−76.9 (8)
O1B—C1B—C8B—C9B	35.3 (3)	O1D—C1D—C8D—C9D	−140.6 (9)
C2B—C1B—C8B—C9B	153.1 (2)	C2D—C1D—C8D—C9D	−22.1 (10)
C14B—C1B—C8B—C9B	−82.8 (3)	C14D—C1D—C8D—C9D	101.6 (9)
C13B—C8B—C9B—C10B	1.5 (5)	C13D—C8D—C9D—C10D	1.9 (14)
C1B—C8B—C9B—C10B	178.5 (4)	C1D—C8D—C9D—C10D	−176.6 (9)
C8B—C9B—C10B—C11B	−3.4 (9)	C8D—C9D—C10D—C11D	−3.5 (16)
C9B—C10B—C11B—C12B	3.7 (12)	C9D—C10D—C11D—C12D	8 (2)
C10B—C11B—C12B—C13B	−2.0 (12)	C10D—C11D—C12D—C13D	−11 (3)
C9B—C8B—C13B—C12B	0.1 (7)	C9D—C8D—C13D—C12D	−4.9 (16)
C1B—C8B—C13B—C12B	−176.9 (5)	C1D—C8D—C13D—C12D	173.7 (10)
C11B—C12B—C13B—C8B	0.2 (11)	C11D—C12D—C13D—C8D	9 (2)
O1B—C1B—C14B—C15B	42.8 (4)	O1D—C1D—C14D—C15D	29.5 (8)
C8B—C1B—C14B—C15B	161.5 (3)	C2D—C1D—C14D—C15D	−89.7 (7)
C2B—C1B—C14B—C15B	−74.1 (3)	C8D—C1D—C14D—C15D	145.9 (6)
O1B—C1B—C14B—C19B	−139.0 (4)	O1D—C1D—C14D—C19D	−149.5 (12)
C8B—C1B—C14B—C19B	−20.3 (5)	C2D—C1D—C14D—C19D	91.4 (13)
C2B—C1B—C14B—C19B	104.1 (5)	C8D—C1D—C14D—C19D	−33.0 (13)
C19B—C14B—C15B—C16B	−1.9 (6)	C19D—C14D—C15D—C16D	−1.7 (14)
C1B—C14B—C15B—C16B	176.4 (4)	C1D—C14D—C15D—C16D	179.4 (10)
C14B—C15B—C16B—C17B	0.3 (8)	C14D—C15D—C16D—C17D	−2.7 (19)
C15B—C16B—C17B—C18B	0.9 (8)	C15D—C16D—C17D—C18D	5 (3)
C16B—C17B—C18B—C19B	−0.4 (7)	C16D—C17D—C18D—C19D	−3 (3)
C17B—C18B—C19B—C14B	−1.4 (8)	C15D—C14D—C19D—C18D	4 (3)

C15B—C14B—C19B—C18B	2.5 (8)	C1D—C14D—C19D—C18D	−177.3 (16)
C1B—C14B—C19B—C18B	−175.8 (4)	C17D—C18D—C19D—C14D	−2 (3)

Symmetry codes: (i) −y+1, x−y, z; (ii) −x+y+1, −x+1, z.

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
O1A—H1A···O1B	0.85	2.33	2.869 (3)	121
O1B—H1BA···O1A	0.84	2.27	2.869 (3)	129
O1B—H1BB···O1B^i	0.82	2.21	2.869 (3)	138
O1B—H1BC···O1B^ii	0.86	2.24	2.869 (3)	130
O1C—H1C···O1D	0.85	2.22	2.856 (7)	131
O1D—H1DA···O1C	0.84	2.24	2.856 (7)	131
O1D—H1DB···O1D^ii	0.82	2.38	2.951 (8)	127
O1D—H1DC···O1D^i	0.85	2.33	2.951 (8)	131

Symmetry codes: (i) −y+1, x−y, z; (ii) −x+y+1, −x+1, z.

Triphenylmethanol (295K_data)

Crystal data

$C_{19}H_{16}O$	Melting point: 433 K
$M_r = 260.32$	Ag $K\alpha$ radiation, $\lambda = 0.56083$ Å
Trigonal, $R\bar{3}{:}H$	Cell parameters from 22044 reflections
$a = 19.3309$ (8) Å	$\theta = 2.3–23.6°$
$c = 26.8542$ (11) Å	$\mu = 0.05$ mm$^{−1}$
$V = 8690.5$ (8) Å^3	$T = 295$ K
$Z = 24$	Prism, colourless
$F(000) = 3312$	$0.38 \times 0.33 \times 0.33$ mm
$D_x = 1.194$ Mg m$^{−3}$	

Data collection

Stoe Stadivari diffractometer	$T_{min} = 0.558$, $T_{max} = 1.000$
	72080 measured reflections
Radiation source: Sealed X-ray tube, Axo Astix-f Microfocus source	4523 independent reflections
	1656 reflections with $I > 2\sigma(I)$
Graded multilayer mirror monochromator	$R_{int} = 0.108$
Detector resolution: 5.81 pixels mm^{-1}	$\theta_{max} = 21.5°$, $\theta_{min} = 2.3°$
ω scans	$h = −25\rightarrow25$
Absorption correction: multi-scan (X-AREA; Stoe & Cie, 2018)	$k = −25\rightarrow25$
	$l = −35\rightarrow35$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.063$	Hydrogen site location: mixed
$wR(F^2) = 0.242$	H-atom parameters constrained
$S = 0.99$	$w = 1/[\sigma^2(F_o^2) + (0.1204P)^2]$
4523 reflections	where $P = (F_o^2 + 2F_c^2)/3$
483 parameters	$(\Delta/\sigma)_{max} < 0.001$
279 restraints	$\Delta\rho_{max} = 0.11$ e Å$^{−3}$
0 constraints	$\Delta\rho_{min} = −0.14$ e Å$^{−3}$
Primary atom site location: dual	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1A	0.666667	0.333333	0.51270 (12)	0.0914 (13)	0.761 (3)
H1A	0.694157	0.379899	0.524947	0.137*	0.2537 (10)
C1A	0.666667	0.333333	0.45924 (16)	0.0615 (13)	0.761 (3)
C2A	0.58276 (19)	0.31029 (19)	0.44168 (11)	0.0616 (8)	0.761 (3)
C3A	0.5387 (2)	0.3366 (3)	0.46772 (14)	0.0858 (11)	0.761 (3)
H3A	0.559553	0.366478	0.496593	0.103*	0.761 (3)
C4A	0.4638 (6)	0.3188 (7)	0.4513 (4)	0.116 (3)	0.761 (3)
H4A	0.434020	0.336006	0.469166	0.140*	0.761 (3)
C5A	0.4335 (5)	0.2751 (6)	0.4078 (4)	0.114 (4)	0.761 (3)
H5A	0.383723	0.264142	0.396160	0.137*	0.761 (3)
C6A	0.4756 (5)	0.2482 (6)	0.3821 (3)	0.103 (3)	0.761 (3)
H6A	0.454732	0.218150	0.353258	0.124*	0.761 (3)
C7A	0.5496 (5)	0.2659 (5)	0.3991 (2)	0.0808 (16)	0.761 (3)
H7A	0.578390	0.247372	0.381366	0.097*	0.761 (3)
O1B	0.76514 (12)	0.36549 (16)	0.60145 (9)	0.0946 (8)	0.761 (3)
H1BA	0.763528	0.369221	0.571207	0.142*	0.2537 (10)
H1BB	0.746050	0.388243	0.617060	0.142*	0.2537 (10)
H1BC	0.737008	0.315795	0.608270	0.142*	0.2537 (10)
C1B	0.84285 (16)	0.38706 (18)	0.62055 (11)	0.0643 (8)	0.761 (3)
C2B	0.86564 (17)	0.32722 (19)	0.60004 (11)	0.0676 (9)	0.761 (3)
C3B	0.8507 (3)	0.3045 (3)	0.55144 (14)	0.1096 (14)	0.761 (3)
H3B	0.824550	0.323452	0.531406	0.131*	0.761 (3)
C4B	0.8743 (6)	0.2535 (8)	0.5317 (3)	0.139 (4)	0.761 (3)
H4B	0.864501	0.239071	0.498283	0.167*	0.761 (3)
C5B	0.9102 (6)	0.2251 (5)	0.5595 (3)	0.122 (3)	0.761 (3)
H5B	0.926576	0.191734	0.545315	0.146*	0.761 (3)
C6B	0.9238 (5)	0.2436 (6)	0.6083 (3)	0.117 (3)	0.761 (3)
H6B	0.947295	0.221585	0.628218	0.140*	0.761 (3)
C7B	0.9019 (4)	0.2963 (4)	0.6283 (3)	0.0942 (19)	0.761 (3)
H7B	0.912232	0.310638	0.661646	0.113*	0.761 (3)
C8B	0.90054 (18)	0.47139 (19)	0.60328 (12)	0.0690 (9)	0.761 (3)
C9B	0.8767 (2)	0.5277 (2)	0.59935 (15)	0.0889 (11)	0.761 (3)
H9B	0.823725	0.512459	0.605925	0.107*	0.761 (3)
C10B	0.9287 (7)	0.6052 (4)	0.5861 (3)	0.114 (3)	0.761 (3)
H10B	0.910946	0.641732	0.583345	0.137*	0.761 (3)
C11B	1.0068 (7)	0.6283 (5)	0.5769 (4)	0.135 (4)	0.761 (3)
H11B	1.042807	0.681234	0.568895	0.162*	0.761 (3)
C12B	1.0322 (4)	0.5740 (5)	0.5793 (4)	0.149 (4)	0.761 (3)
H12B	1.085032	0.589464	0.572045	0.179*	0.761 (3)
C13B	0.9792 (3)	0.4963 (3)	0.5927 (2)	0.1009 (17)	0.761 (3)
H13B	0.997098	0.459746	0.594685	0.121*	0.761 (3)
C14B	0.8371 (2)	0.3825 (2)	0.67749 (13)	0.0613 (8)	0.761 (3)
C15B	0.7720 (2)	0.3181 (3)	0.69901 (15)	0.0925 (12)	0.761 (3)
H15B	0.731546	0.280294	0.678923	0.111*	0.761 (3)
C16B	0.7663 (4)	0.3092 (5)	0.7500 (3)	0.100 (2)	0.761 (3)

H16B	0.722188	0.265369	0.764060	0.120*	0.761 (3)
C17B	0.8247 (4)	0.3639 (4)	0.77990 (19)	0.0905 (16)	0.761 (3)
H17B	0.821027	0.357339	0.814286	0.109*	0.761 (3)
C18B	0.8887 (3)	0.4284 (3)	0.75912 (17)	0.0960 (15)	0.761 (3)
H18B	0.929017	0.466024	0.779317	0.115*	0.761 (3)
C19B	0.8936 (3)	0.4378 (4)	0.7080 (2)	0.0756 (15)	0.761 (3)
H19B	0.936631	0.483054	0.694220	0.091*	0.761 (3)
O1C	0.666667	0.333333	0.6444 (5)	0.096 (4)	0.239 (3)
H1C	0.682444	0.378577	0.630954	0.144*	0.0797 (10)
C1C	0.666667	0.333333	0.6968 (6)	0.067 (4)	0.239 (3)
C2C	0.7494 (7)	0.3565 (7)	0.7159 (5)	0.086 (3)	0.239 (3)
C3C	0.7614 (16)	0.3248 (15)	0.7597 (8)	0.124 (11)	0.239 (3)
H3C	0.718063	0.289797	0.779120	0.148*	0.239 (3)
C4C	0.8382 (16)	0.3459 (18)	0.7740 (10)	0.190 (16)	0.239 (3)
H4C	0.847018	0.325127	0.803037	0.228*	0.239 (3)
C5C	0.9014 (13)	0.3981 (14)	0.7447 (11)	0.171 (11)	0.239 (3)
H5C	0.952844	0.411478	0.754391	0.206*	0.239 (3)
C6C	0.8922 (13)	0.431 (2)	0.7026 (13)	0.174 (16)	0.239 (3)
H6C	0.936126	0.466658	0.683861	0.208*	0.239 (3)
C7C	0.8161 (8)	0.4091 (9)	0.6883 (6)	0.105 (5)	0.239 (3)
H7C	0.808723	0.430334	0.659071	0.126*	0.239 (3)
O1D	0.7407 (5)	0.4307 (4)	0.5563 (3)	0.104 (3)	0.239 (3)
H1DA	0.735152	0.429060	0.586798	0.156*	0.0797 (10)
H1DB	0.754328	0.398510	0.546886	0.156*	0.0797 (10)
H1DC	0.696732	0.418001	0.543089	0.156*	0.0797 (10)
C1D	0.7984 (6)	0.5107 (5)	0.5410 (4)	0.074 (2)	0.239 (3)
C2D	0.7747 (6)	0.5696 (6)	0.5642 (3)	0.074 (3)	0.239 (3)
C3D	0.7567 (9)	0.5648 (8)	0.6131 (4)	0.122 (5)	0.239 (3)
H3D	0.755580	0.524072	0.632119	0.146*	0.239 (3)
C4D	0.7398 (13)	0.6189 (14)	0.6353 (10)	0.124 (10)	0.239 (3)
H4D	0.728498	0.614212	0.669221	0.149*	0.239 (3)
C5D	0.7391 (18)	0.6777 (17)	0.6098 (11)	0.112 (8)	0.239 (3)
H5D	0.728146	0.714530	0.624757	0.134*	0.239 (3)
C6D	0.756 (3)	0.6801 (19)	0.5606 (12)	0.23 (2)	0.239 (3)
H6D	0.760372	0.722931	0.542143	0.270*	0.239 (3)
C7D	0.766 (2)	0.6232 (19)	0.5360 (10)	0.109 (10)	0.239 (3)
H7D	0.766762	0.621529	0.501386	0.130*	0.239 (3)
C8D	0.8812 (6)	0.5292 (6)	0.5580 (4)	0.073 (3)	0.239 (3)
C9D	0.9417 (15)	0.6018 (12)	0.5772 (8)	0.120 (10)	0.239 (3)
H9D	0.931304	0.643600	0.580757	0.143*	0.239 (3)
C10D	1.0155 (15)	0.6146 (15)	0.5909 (8)	0.105 (7)	0.239 (3)
H10D	1.054059	0.664218	0.603007	0.126*	0.239 (3)
C11D	1.0319 (15)	0.5536 (16)	0.5866 (10)	0.132 (9)	0.239 (3)
H11D	1.079899	0.559758	0.598487	0.159*	0.239 (3)
C12D	0.9767 (11)	0.4832 (13)	0.5647 (6)	0.124 (7)	0.239 (3)
H12D	0.990107	0.445364	0.554674	0.149*	0.239 (3)
C13D	0.9009 (8)	0.4708 (7)	0.5581 (7)	0.113 (5)	0.239 (3)
H13D	0.859930	0.418489	0.553273	0.136*	0.239 (3)

C14D	0.7968 (6)	0.5122 (7)	0.4824 (4)	0.076 (3)	0.239 (3)
C15D	0.7274 (7)	0.4662 (7)	0.4579 (5)	0.101 (4)	0.239 (3)
H15D	0.681858	0.431590	0.475739	0.122*	0.239 (3)
C16D	0.7233 (16)	0.4698 (16)	0.4069 (8)	0.109 (9)	0.239 (3)
H16D	0.675128	0.438305	0.390548	0.131*	0.239 (3)
C17D	0.7902 (15)	0.5197 (17)	0.3806 (7)	0.087 (6)	0.239 (3)
H17D	0.788042	0.520924	0.345998	0.104*	0.239 (3)
C18D	0.8597 (15)	0.5677 (16)	0.4045 (7)	0.086 (6)	0.239 (3)
H18D	0.904107	0.605123	0.386849	0.103*	0.239 (3)
C19D	0.8642 (12)	0.5605 (17)	0.4559 (7)	0.102 (8)	0.239 (3)
H19D	0.913176	0.588580	0.472064	0.122*	0.239 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.117 (2)	0.117 (2)	0.040 (2)	0.0584 (10)	0.000	0.000
C1A	0.072 (2)	0.072 (2)	0.040 (2)	0.0362 (10)	0.000	0.000
C2A	0.0617 (19)	0.0650 (19)	0.0534 (17)	0.0281 (16)	0.0058 (14)	0.0045 (14)
C3A	0.078 (3)	0.091 (3)	0.092 (3)	0.044 (2)	0.014 (2)	−0.007 (2)
C4A	0.091 (5)	0.117 (5)	0.157 (7)	0.063 (4)	0.027 (4)	−0.002 (4)
C5A	0.057 (3)	0.103 (7)	0.166 (8)	0.028 (3)	−0.012 (4)	0.026 (4)
C6A	0.081 (4)	0.097 (7)	0.122 (5)	0.037 (4)	−0.031 (4)	−0.015 (4)
C7A	0.073 (3)	0.091 (4)	0.076 (3)	0.039 (3)	−0.006 (3)	−0.008 (3)
O1B	0.0541 (13)	0.131 (2)	0.0955 (18)	0.0443 (14)	−0.0238 (11)	−0.0075 (14)
C1B	0.0453 (15)	0.083 (2)	0.0640 (18)	0.0313 (15)	−0.0102 (13)	−0.0049 (15)
C2B	0.0574 (18)	0.077 (2)	0.0620 (19)	0.0289 (17)	−0.0053 (14)	−0.0049 (15)
C3B	0.148 (4)	0.127 (4)	0.075 (3)	0.085 (3)	−0.015 (2)	−0.018 (2)
C4B	0.209 (12)	0.162 (9)	0.089 (4)	0.125 (9)	−0.016 (5)	−0.031 (4)
C5B	0.162 (8)	0.122 (4)	0.116 (5)	0.096 (5)	0.022 (5)	−0.013 (4)
C6B	0.149 (7)	0.146 (8)	0.105 (5)	0.111 (7)	−0.006 (5)	−0.010 (5)
C7B	0.115 (4)	0.116 (5)	0.081 (3)	0.080 (4)	−0.013 (3)	−0.020 (3)
C8B	0.0591 (19)	0.082 (2)	0.063 (2)	0.0330 (17)	−0.0030 (15)	0.0023 (17)
C9B	0.097 (3)	0.098 (3)	0.084 (3)	0.059 (3)	0.002 (2)	0.007 (2)
C10B	0.151 (7)	0.106 (5)	0.107 (4)	0.080 (5)	0.014 (4)	0.024 (3)
C11B	0.153 (9)	0.098 (4)	0.128 (8)	0.043 (5)	0.018 (6)	0.034 (4)
C12B	0.098 (5)	0.115 (5)	0.214 (10)	0.038 (4)	0.057 (5)	0.036 (5)
C13B	0.069 (3)	0.086 (3)	0.141 (5)	0.033 (2)	0.023 (3)	0.018 (3)
C14B	0.050 (2)	0.074 (2)	0.0629 (19)	0.0335 (18)	−0.0025 (15)	−0.0024 (16)
C15B	0.071 (2)	0.096 (3)	0.081 (3)	0.020 (2)	−0.0015 (19)	−0.009 (2)
C16B	0.090 (4)	0.101 (4)	0.078 (3)	0.026 (3)	0.020 (3)	0.011 (3)
C17B	0.108 (5)	0.113 (4)	0.056 (2)	0.059 (3)	0.004 (3)	0.002 (2)
C18B	0.101 (3)	0.095 (3)	0.073 (2)	0.035 (3)	−0.022 (2)	−0.013 (2)
C19B	0.066 (3)	0.078 (3)	0.064 (2)	0.022 (2)	−0.013 (2)	−0.001 (2)
O1C	0.112 (6)	0.112 (6)	0.063 (6)	0.056 (3)	0.000	0.000
C1C	0.070 (5)	0.070 (5)	0.063 (7)	0.035 (3)	0.000	0.000
C2C	0.088 (6)	0.083 (8)	0.086 (7)	0.043 (6)	−0.017 (5)	−0.016 (6)
C3C	0.129 (13)	0.17 (2)	0.103 (16)	0.102 (16)	−0.009 (12)	0.019 (16)
C4C	0.132 (15)	0.18 (3)	0.23 (3)	0.059 (18)	−0.094 (16)	0.00 (2)

C5C	0.090 (11)	0.132 (19)	0.27 (3)	0.035 (11)	−0.081 (13)	−0.049 (16)
C6C	0.095 (12)	0.21 (4)	0.21 (3)	0.080 (19)	−0.018 (17)	−0.03 (2)
C7C	0.086 (8)	0.107 (11)	0.127 (12)	0.051 (8)	0.014 (8)	0.020 (8)
O1D	0.091 (5)	0.070 (4)	0.125 (7)	0.021 (4)	0.011 (5)	0.030 (4)
C1D	0.065 (5)	0.051 (5)	0.092 (6)	0.018 (4)	0.005 (4)	0.014 (4)
C2D	0.068 (6)	0.067 (6)	0.075 (6)	0.026 (5)	0.004 (5)	0.015 (4)
C3D	0.163 (14)	0.136 (11)	0.088 (7)	0.091 (11)	0.053 (9)	0.044 (7)
C4D	0.13 (2)	0.15 (2)	0.110 (13)	0.087 (19)	0.037 (14)	0.012 (12)
C5D	0.077 (11)	0.153 (19)	0.130 (15)	0.077 (14)	−0.016 (10)	−0.013 (13)
C6D	0.43 (7)	0.19 (3)	0.16 (2)	0.24 (4)	0.10 (3)	0.06 (2)
C7D	0.131 (19)	0.12 (2)	0.119 (14)	0.10 (2)	0.049 (14)	0.049 (15)
C8D	0.071 (5)	0.077 (6)	0.071 (7)	0.036 (5)	0.008 (5)	0.010 (5)
C9D	0.084 (10)	0.117 (13)	0.14 (2)	0.041 (10)	−0.018 (13)	−0.028 (14)
C10D	0.077 (9)	0.142 (19)	0.059 (9)	0.028 (12)	−0.004 (7)	−0.010 (12)
C11D	0.134 (17)	0.20 (2)	0.081 (12)	0.098 (15)	−0.037 (13)	0.005 (13)
C12D	0.135 (11)	0.191 (17)	0.086 (12)	0.111 (12)	−0.018 (10)	−0.019 (11)
C13D	0.099 (8)	0.087 (8)	0.156 (14)	0.049 (7)	−0.002 (9)	0.005 (8)
C14D	0.066 (6)	0.068 (7)	0.091 (6)	0.032 (5)	0.007 (4)	0.010 (5)
C15D	0.088 (8)	0.084 (9)	0.109 (8)	0.026 (7)	−0.011 (6)	0.001 (7)
C16D	0.103 (13)	0.12 (2)	0.117 (10)	0.061 (13)	−0.034 (9)	−0.017 (11)
C17D	0.136 (14)	0.091 (12)	0.063 (8)	0.079 (12)	−0.020 (7)	−0.031 (7)
C18D	0.088 (11)	0.131 (15)	0.066 (8)	0.075 (10)	0.006 (6)	0.001 (7)
C19D	0.094 (10)	0.13 (2)	0.068 (8)	0.048 (10)	0.012 (7)	0.032 (10)

Geometric parameters (Å, º)

O1A—C1A	1.436 (5)	O1C—C1C	1.407 (19)
O1A—H1A	0.8500	O1C—H1C	0.8500
O1A—H1A[i]	0.8500	O1C—H1C[i]	0.8501
O1A—H1A[ii]	0.8501	O1C—H1C[ii]	0.8501
C1A—C2A[i]	1.526 (3)	C1C—C2C	1.518 (12)
C1A—C2A[ii]	1.526 (3)	C1C—C2C[ii]	1.518 (12)
C1A—C2A	1.526 (3)	C1C—C2C[i]	1.518 (12)
C2A—C7A	1.380 (7)	C2C—C7C	1.391 (14)
C2A—C3A	1.380 (5)	C2C—C3C	1.399 (18)
C3A—C4A	1.383 (10)	C3C—C4C	1.38 (2)
C3A—H3A	0.9300	C3C—H3C	0.9300
C4A—C5A	1.388 (11)	C4C—C5C	1.38 (2)
C4A—H4A	0.9300	C4C—H4C	0.9300
C5A—C6A	1.354 (10)	C5C—C6C	1.35 (2)
C5A—H5A	0.9300	C5C—H5C	0.9300
C6A—C7A	1.371 (9)	C6C—C7C	1.368 (19)
C6A—H6A	0.9300	C6C—H6C	0.9300
C7A—H7A	0.9300	C7C—H7C	0.9300
O1B—C1B	1.438 (3)	O1D—C1D	1.442 (11)
O1B—H1BA	0.8172	O1D—H1DA	0.8254
O1B—H1BB	0.8171	O1D—H1DB	0.8264
O1B—H1BC	0.8543	O1D—H1DC	0.8364

C1B—C8B	1.516 (4)	C1D—C8D	1.524 (14)
C1B—C2B	1.531 (4)	C1D—C2D	1.554 (14)
C1B—C14B	1.532 (4)	C1D—C14D	1.575 (15)
C2B—C7B	1.357 (7)	C2D—C3D	1.350 (12)
C2B—C3B	1.361 (4)	C2D—C7D	1.361 (19)
C3B—C4B	1.382 (12)	C3D—C4D	1.38 (2)
C3B—H3B	0.9300	C3D—H3D	0.9300
C4B—C5B	1.312 (11)	C4D—C5D	1.33 (2)
C4B—H4B	0.9300	C4D—H4D	0.9300
C5B—C6B	1.351 (7)	C5D—C6D	1.355 (17)
C5B—H5B	0.9300	C5D—H5D	0.9300
C6B—C7B	1.392 (9)	C6D—C7D	1.38 (2)
C6B—H6B	0.9300	C6D—H6D	0.9300
C7B—H7B	0.9300	C7D—H7D	0.9300
C8B—C13B	1.376 (5)	C8D—C13D	1.360 (13)
C8B—C9B	1.381 (5)	C8D—C9D	1.402 (18)
C9B—C10B	1.370 (9)	C9D—C10D	1.37 (2)
C9B—H9B	0.9300	C9D—H9D	0.9300
C10B—C11B	1.366 (11)	C10D—C11D	1.37 (2)
C10B—H10B	0.9300	C10D—H10D	0.9300
C11B—C12B	1.364 (9)	C11D—C12D	1.37 (2)
C11B—H11B	0.9300	C11D—H11D	0.9300
C12B—C13B	1.378 (9)	C12D—C13D	1.372 (16)
C12B—H12B	0.9300	C12D—H12D	0.9300
C13B—H13B	0.9300	C13D—H13D	0.9300
C14B—C19B	1.356 (7)	C14D—C15D	1.353 (13)
C14B—C15B	1.379 (5)	C14D—C19D	1.365 (18)
C15B—C16B	1.378 (8)	C15D—C16D	1.374 (19)
C15B—H15B	0.9300	C15D—H15D	0.9300
C16B—C17B	1.357 (9)	C16D—C17D	1.36 (2)
C16B—H16B	0.9300	C16D—H16D	0.9300
C17B—C18B	1.361 (7)	C17D—C18D	1.355 (19)
C17B—H17B	0.9300	C17D—H17D	0.9300
C18B—C19B	1.382 (7)	C18D—C19D	1.393 (18)
C18B—H18B	0.9300	C18D—H18D	0.9300
C19B—H19B	0.9300	C19D—H19D	0.9300
C1A—O1A—H1A	112.8	C14B—C19B—H19B	119.3
C1A—O1A—H1A[i]	112.764 (1)	C18B—C19B—H19B	119.3
C1A—O1A—H1A[ii]	112.760 (1)	C1C—O1C—H1C	115.2
H1A—O1A—H1A[i]	106.0	C1C—O1C—H1C[i]	115.240 (4)
H1A—O1A—H1A[ii]	106.0	H1C—O1C—H1C[i]	103.1
H1A[i]—O1A—H1A[ii]	106.0	O1C—C1C—C2C	109.7 (7)
O1A—C1A—C2A[i]	108.00 (19)	O1C—C1C—C2C[ii]	109.7 (7)
O1A—C1A—C2A[ii]	108.00 (19)	C2C—C1C—C2C[ii]	109.3 (8)
C2A[i]—C1A—C2A[ii]	110.91 (18)	O1C—C1C—C2C[i]	109.7 (7)
O1A—C1A—C2A	108.00 (19)	C2C—C1C—C2C[i]	109.3 (8)
C2A[i]—C1A—C2A	110.91 (18)	C2C[ii]—C1C—C2C[i]	109.3 (8)

C2Aⁱⁱ—C1A—C2A	110.90 (18)	C7C—C2C—C3C	118.1 (14)
C7A—C2A—C3A	117.9 (4)	C7C—C2C—C1C	119.4 (11)
C7A—C2A—C1A	122.2 (4)	C3C—C2C—C1C	122.4 (14)
C3A—C2A—C1A	119.8 (3)	C4C—C3C—C2C	119.6 (19)
C2A—C3A—C4A	120.6 (5)	C4C—C3C—H3C	120.2
C2A—C3A—H3A	119.7	C2C—C3C—H3C	120.2
C4A—C3A—H3A	119.7	C5C—C4C—C3C	119 (2)
C3A—C4A—C5A	119.4 (7)	C5C—C4C—H4C	120.5
C3A—C4A—H4A	120.3	C3C—C4C—H4C	120.5
C5A—C4A—H4A	120.3	C6C—C5C—C4C	123.1 (19)
C6A—C5A—C4A	120.7 (7)	C6C—C5C—H5C	118.5
C6A—C5A—H5A	119.6	C4C—C5C—H5C	118.5
C4A—C5A—H5A	119.6	C5C—C6C—C7C	118 (2)
C5A—C6A—C7A	119.1 (8)	C5C—C6C—H6C	121.2
C5A—C6A—H6A	120.5	C7C—C6C—H6C	121.2
C7A—C6A—H6A	120.5	C6C—C7C—C2C	122.5 (16)
C6A—C7A—C2A	122.3 (7)	C6C—C7C—H7C	118.7
C6A—C7A—H7A	118.9	C2C—C7C—H7C	118.7
C2A—C7A—H7A	118.9	C1D—O1D—H1DA	109.8
C1B—O1B—H1BA	114.2	C1D—O1D—H1DB	110.7
C1B—O1B—H1BB	110.4	C1D—O1D—H1DC	108.8
C1B—O1B—H1BC	103.6	H1DA—O1D—H1DB	111.0
H1BA—O1B—H1BB	114.5	H1DA—O1D—H1DC	108.4
H1BA—O1B—H1BC	106.3	H1DB—O1D—H1DC	108.1
H1BB—O1B—H1BC	106.9	O1D—C1D—C8D	109.0 (8)
C1B—O1B—H1Cⁱⁱ	119.5 (4)	O1D—C1D—C2D	108.6 (8)
O1B—C1B—C8B	107.6 (2)	C8D—C1D—C2D	111.6 (8)
O1B—C1B—C2B	107.8 (2)	O1D—C1D—C14D	107.0 (8)
C8B—C1B—C2B	111.6 (2)	C8D—C1D—C14D	108.9 (8)
O1B—C1B—C14B	107.7 (2)	C2D—C1D—C14D	111.7 (8)
C8B—C1B—C14B	111.1 (3)	C3D—C2D—C7D	117.8 (14)
C2B—C1B—C14B	110.8 (3)	C3D—C2D—C1D	120.0 (9)
C7B—C2B—C3B	117.8 (4)	C7D—C2D—C1D	122.1 (13)
C7B—C2B—C1B	122.6 (4)	C2D—C3D—C4D	121.4 (15)
C3B—C2B—C1B	119.6 (3)	C2D—C3D—H3D	119.3
C2B—C3B—C4B	120.4 (5)	C4D—C3D—H3D	119.3
C2B—C3B—H3B	119.8	C5D—C4D—C3D	122 (2)
C4B—C3B—H3B	119.8	C5D—C4D—H4D	119.0
C5B—C4B—C3B	120.8 (7)	C3D—C4D—H4D	119.0
C5B—C4B—H4B	119.6	C4D—C5D—C6D	115 (2)
C3B—C4B—H4B	119.6	C4D—C5D—H5D	122.3
C4B—C5B—C6B	121.0 (8)	C6D—C5D—H5D	122.3
C4B—C5B—H5B	119.5	C5D—C6D—C7D	124 (2)
C6B—C5B—H5B	119.5	C5D—C6D—H6D	117.8
C5B—C6B—C7B	118.5 (7)	C7D—C6D—H6D	117.8
C5B—C6B—H6B	120.8	C2D—C7D—C6D	118 (2)
C7B—C6B—H6B	120.8	C2D—C7D—H7D	121.2
C2B—C7B—C6B	121.4 (6)	C6D—C7D—H7D	121.2

C2B—C7B—H7B	119.3	C13D—C8D—C9D	113.0 (14)
C6B—C7B—H7B	119.3	C13D—C8D—C1D	120.2 (10)
C13B—C8B—C9B	117.0 (4)	C9D—C8D—C1D	126.7 (14)
C13B—C8B—C1B	122.0 (3)	C10D—C9D—C8D	124 (2)
C9B—C8B—C1B	121.0 (3)	C10D—C9D—H9D	118.2
C10B—C9B—C8B	122.0 (6)	C8D—C9D—H9D	118.2
C10B—C9B—H9B	119.0	C9D—C10D—C11D	119 (2)
C8B—C9B—H9B	119.0	C9D—C10D—H10D	120.4
C11B—C10B—C9B	119.4 (8)	C11D—C10D—H10D	120.4
C11B—C10B—H10B	120.3	C10D—C11D—C12D	119.2 (19)
C9B—C10B—H10B	120.3	C10D—C11D—H11D	120.4
C12B—C11B—C10B	120.2 (8)	C12D—C11D—H11D	120.4
C12B—C11B—H11B	119.9	C13D—C12D—C11D	117.5 (17)
C10B—C11B—H11B	119.9	C13D—C12D—H12D	121.2
C11B—C12B—C13B	119.6 (7)	C11D—C12D—H12D	121.2
C11B—C12B—H12B	120.2	C8D—C13D—C12D	124.9 (14)
C13B—C12B—H12B	120.2	C8D—C13D—H13D	117.5
C8B—C13B—C12B	121.6 (5)	C12D—C13D—H13D	117.5
C8B—C13B—H13B	119.2	C15D—C14D—C19D	119.3 (13)
C12B—C13B—H13B	119.2	C15D—C14D—C1D	119.9 (10)
C19B—C14B—C15B	118.1 (4)	C19D—C14D—C1D	120.9 (11)
C19B—C14B—C1B	123.4 (3)	C14D—C15D—C16D	121.0 (15)
C15B—C14B—C1B	118.5 (3)	C14D—C15D—H15D	119.5
C16B—C15B—C14B	120.6 (4)	C16D—C15D—H15D	119.5
C16B—C15B—H15B	119.7	C17D—C16D—C15D	120 (2)
C14B—C15B—H15B	119.7	C17D—C16D—H16D	120.2
C17B—C16B—C15B	120.5 (5)	C15D—C16D—H16D	120.2
C17B—C16B—H16B	119.8	C18D—C17D—C16D	120.2 (18)
C15B—C16B—H16B	119.8	C18D—C17D—H17D	119.9
C16B—C17B—C18B	119.5 (5)	C16D—C17D—H17D	119.9
C16B—C17B—H17B	120.3	C17D—C18D—C19D	119.5 (18)
C18B—C17B—H17B	120.3	C17D—C18D—H18D	120.2
C17B—C18B—C19B	120.0 (5)	C19D—C18D—H18D	120.2
C17B—C18B—H18B	120.0	C14D—C19D—C18D	119.9 (18)
C19B—C18B—H18B	120.0	C14D—C19D—H19D	120.0
C14B—C19B—C18B	121.3 (4)	C18D—C19D—H19D	120.0
O1A—C1A—C2A—C7A	−145.6 (5)	O1C—C1C—C2C—C7C	31.7 (13)
C2A^i—C1A—C2A—C7A	−27.4 (6)	C2C^ii—C1C—C2C—C7C	151.9 (13)
C2A^ii—C1A—C2A—C7A	96.3 (5)	C2C^i—C1C—C2C—C7C	−88.6 (18)
O1A—C1A—C2A—C3A	36.8 (3)	O1C—C1C—C2C—C3C	−146.3 (13)
C2A^i—C1A—C2A—C3A	155.0 (3)	C2C^ii—C1C—C2C—C3C	−26.0 (18)
C2A^ii—C1A—C2A—C3A	−81.3 (5)	C2C^i—C1C—C2C—C3C	93.5 (14)
C7A—C2A—C3A—C4A	−0.2 (8)	C7C—C2C—C3C—C4C	−0.5 (17)
C1A—C2A—C3A—C4A	177.5 (6)	C1C—C2C—C3C—C4C	177.4 (15)
C2A—C3A—C4A—C5A	−0.9 (11)	C2C—C3C—C4C—C5C	0 (2)
C3A—C4A—C5A—C6A	1.5 (14)	C3C—C4C—C5C—C6C	1 (4)
C4A—C5A—C6A—C7A	−1.1 (14)	C4C—C5C—C6C—C7C	−1 (5)

C5A—C6A—C7A—C2A	0.0 (13)	C5C—C6C—C7C—C2C	1 (5)
C3A—C2A—C7A—C6A	0.6 (10)	C3C—C2C—C7C—C6C	0 (3)
C1A—C2A—C7A—C6A	−177.0 (6)	C1C—C2C—C7C—C6C	−178 (3)
O1B—C1B—C2B—C7B	−138.5 (4)	O1D—C1D—C2D—C3D	48.5 (13)
C8B—C1B—C2B—C7B	103.5 (5)	C8D—C1D—C2D—C3D	−71.6 (13)
C14B—C1B—C2B—C7B	−20.9 (5)	C14D—C1D—C2D—C3D	166.2 (10)
O1B—C1B—C2B—C3B	42.6 (4)	O1D—C1D—C2D—C7D	−127 (2)
C8B—C1B—C2B—C3B	−75.3 (4)	C8D—C1D—C2D—C7D	113 (2)
C14B—C1B—C2B—C3B	160.3 (3)	C14D—C1D—C2D—C7D	−9 (2)
C7B—C2B—C3B—C4B	−1.9 (8)	C7D—C2D—C3D—C4D	−8 (2)
C1B—C2B—C3B—C4B	177.0 (6)	C1D—C2D—C3D—C4D	176.3 (12)
C2B—C3B—C4B—C5B	1.0 (13)	C2D—C3D—C4D—C5D	1 (2)
C3B—C4B—C5B—C6B	1.3 (16)	C3D—C4D—C5D—C6D	0 (4)
C4B—C5B—C6B—C7B	−2.7 (14)	C4D—C5D—C6D—C7D	6 (6)
C3B—C2B—C7B—C6B	0.5 (9)	C3D—C2D—C7D—C6D	13 (4)
C1B—C2B—C7B—C6B	−178.3 (6)	C1D—C2D—C7D—C6D	−171 (3)
C5B—C6B—C7B—C2B	1.7 (12)	C5D—C6D—C7D—C2D	−13 (6)
O1B—C1B—C8B—C13B	−147.2 (4)	O1D—C1D—C8D—C13D	35.4 (15)
C2B—C1B—C8B—C13B	−29.1 (5)	C2D—C1D—C8D—C13D	155.3 (11)
C14B—C1B—C8B—C13B	95.1 (4)	C14D—C1D—C8D—C13D	−80.9 (14)
O1B—C1B—C8B—C9B	35.4 (4)	O1D—C1D—C8D—C9D	−140.8 (13)
C2B—C1B—C8B—C9B	153.5 (3)	C2D—C1D—C8D—C9D	−20.8 (16)
C14B—C1B—C8B—C9B	−82.3 (4)	C14D—C1D—C8D—C9D	102.9 (14)
C13B—C8B—C9B—C10B	−0.6 (7)	C13D—C8D—C9D—C10D	4.8 (16)
C1B—C8B—C9B—C10B	176.9 (5)	C1D—C8D—C9D—C10D	−178.8 (13)
C8B—C9B—C10B—C11B	−0.7 (10)	C8D—C9D—C10D—C11D	−1 (2)
C9B—C10B—C11B—C12B	2.1 (14)	C9D—C10D—C11D—C12D	6 (3)
C10B—C11B—C12B—C13B	−2.1 (15)	C10D—C11D—C12D—C13D	−14 (3)
C9B—C8B—C13B—C12B	0.7 (9)	C9D—C8D—C13D—C12D	−15 (2)
C1B—C8B—C13B—C12B	−176.9 (6)	C1D—C8D—C13D—C12D	168.8 (15)
C11B—C12B—C13B—C8B	0.7 (13)	C11D—C12D—C13D—C8D	20 (3)
O1B—C1B—C14B—C19B	−137.9 (5)	O1D—C1D—C14D—C15D	33.3 (14)
C8B—C1B—C14B—C19B	−20.2 (6)	C8D—C1D—C14D—C15D	151.0 (11)
C2B—C1B—C14B—C19B	104.4 (5)	C2D—C1D—C14D—C15D	−85.3 (12)
O1B—C1B—C14B—C15B	43.6 (4)	O1D—C1D—C14D—C19D	−147.8 (18)
C8B—C1B—C14B—C15B	161.2 (3)	C8D—C1D—C14D—C19D	−30.2 (19)
C2B—C1B—C14B—C15B	−74.2 (4)	C2D—C1D—C14D—C19D	93.5 (19)
C19B—C14B—C15B—C16B	−2.2 (8)	C19D—C14D—C15D—C16D	−2.6 (19)
C1B—C14B—C15B—C16B	176.5 (5)	C1D—C14D—C15D—C16D	176.2 (14)
C14B—C15B—C16B—C17B	0.2 (10)	C14D—C15D—C16D—C17D	1 (2)
C15B—C16B—C17B—C18B	0.8 (11)	C15D—C16D—C17D—C18D	−2 (4)
C16B—C17B—C18B—C19B	0.2 (9)	C16D—C17D—C18D—C19D	6 (4)
C15B—C14B—C19B—C18B	3.2 (8)	C15D—C14D—C19D—C18D	6 (4)
C1B—C14B—C19B—C18B	−175.4 (5)	C1D—C14D—C19D—C18D	−173 (2)
C17B—C18B—C19B—C14B	−2.3 (9)	C17D—C18D—C19D—C14D	−8 (4)

Symmetry codes: (i) −*y*+1, *x*−*y*, *z*; (ii) −*x*+*y*+1, −*x*+1, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*A*···O1*B*	0.85	2.56	2.917 (3)	106
O1*B*—H1*BA*···O1*A*	0.82	2.27	2.917 (3)	136
O1*B*—H1*BB*···O1*B*[i]	0.82	2.31	2.912 (3)	131
O1*B*—H1*BC*···O1*B*[ii]	0.85	2.31	2.912 (4)	128
O1*C*—H1*C*···O1*D*	0.85	2.27	2.916 (13)	133
O1*D*—H1*DA*···O1*C*	0.83	2.26	2.916 (13)	136
O1*D*—H1*DB*···O1*D*[ii]	0.83	2.35	2.947 (13)	130
O1*D*—H1*DC*···O1*D*[i]	0.84	2.33	2.947 (13)	132

Symmetry codes: (i) $-y+1, x-y, z$; (ii) $-x+y+1, -x+1, z$.

Comparison between the three X-ray structures of triphenylmethanol determined at room temperature

	1992[a]	1999[b]	2019[c]
Date of publication			
Diffractometer	CAD-4	R-Axis II	Stadivari
Detector	NaI scintillator	Image plate	HPAD[d]
T (K)	294	293	295
No. independent reflections	2467	3448	4523
Refined parameters	253	322	483
Data resolution (Å)	0.89	0.82	0.77
Range for σ(C—C)	0.040–0.007 Å	–	0.020–0.003 Å

Nores and references: (*a*) Ferguson *et al.* (1992); (*b*) Serrano-González *et al.* (1999); (*c*) this work; (*d*) Hybrid Pixel Array Detector.