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2,8,14,20-Tetrakis(4-hydroxyphenyl)-pyrogallol[4]arene dimethylformamide hexasolvate

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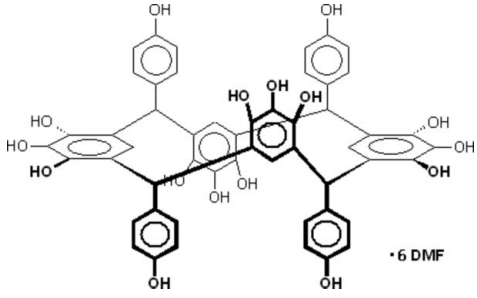
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; disorder in solvent or counterion; R factor = 0.054; wR factor = 0.151; data-to-parameter ratio = 17.2.

The title compound, $C_{52}H_{40}O_{16}\cdot 6C_3H_7NO$, is shown to adopt a macrocyclic chair conformation. The asymmetric unit contains one-half of the main molecule, which lies on a crystallographic inversion center, together with three solvent molecules. Extensive intermolecular O—H···O hydrogen bonding between the hydroxyl groups and dimethylformamide molecules generates a three-dimensional network.

Related literature

For details of calix-shaped compounds and their applications, see: Asfari *et al.* (2001). For related structures, see: Makeiff & Sherman (2005, and references therein), Zambrano *et al.* (2006); Kass *et al.* (2006), Dueno *et al.* (2006) and Cave *et al.* (2005).



Experimental

Crystal data

$C_{52}H_{40}O_{16}\cdot 6C_3H_7NO$
M_r = 1359.42
Triclinic, $P\overline{1}$
a = 10.6481 (5) Å
b = 11.5153 (6) Å
c = 14.3315 (7) Å
α = 75.748 (1)°
β = 78.462 (1)°
γ = 77.891 (1)°
V = 1644.8 (1) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 (2) K
0.44 × 0.25 × 0.19 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS* in *SAINT-Plus*; Bruker, 2003)
T_{min} = 0.914, T_{max} = 0.981
17256 measured reflections
8127 independent reflections
7050 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.151
S = 1.03
8127 reflections
472 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4*B*—H4*BB*···O1^{i}	0.84	2.10	2.923 (2)	168
O3*B*—H3*BB*···O3*D*^{ii}	0.84	1.98	2.7545 (17)	153
O3*B*—H3*BB*···O3^{ii}	0.84	1.98	2.7545 (17)	153
O2*B*—H2*BA*···O2*D*	0.84	1.92	2.7561 (17)	174
O2*B*—H2*BA*···O2	0.84	1.92	2.7561 (17)	174
O1*B*—H1*BB*···O2*D*	0.84	2.00	2.8429 (17)	176
O1*B*—H1*BB*···O2	0.84	2.00	2.8429 (17)	176
O4*A*—H4*AA*···O2*D*^{iii}	0.84	2.48	2.8933 (19)	111
O4*A*—H4*AA*···O2^{iii}	0.84	2.48	2.8933 (19)	111
O3*A*—H3*AB*···O4*B*^{iv}	0.84	1.99	2.7663 (17)	153
O2*A*—H2*AA*···O1^{v}	0.84	1.92	2.7484 (19)	169
O1*A*—H1*AC*···O1^{v}	0.84	1.89	2.7227 (18)	172

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2285).

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supplementary materials

Acta Cryst. (2007). E**63**, o3533-o3534 [**doi:10.1107/S1600536807021071**]

2,8,14,20-Tetrakis(4-hydroxyphenyl)pyrogallol[4]arene dimethylformamide hexasolvate

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Comment

Calix-shaped compounds such as pyrogallolarenes have received considerable attention during the last two decades due to their potential use in a number of industrial applications (Asfari *et al.*, 2001). The conformational isomers of pyrogallol[4]arenes are being studied by various investigators (Makeiff & Sherman, 2005, and references therein). Our investigations have shown that aryl-substituted pyrogallol[4]arenes adopt a chair (rctt) conformation (Zambrano *et al.*, 2006; Kass *et al.*, 2006), whereas alkyl substituents lead to the crown (rccc) structure (Dueno *et al.*, 2006). Here, we report the crystal structure of the compound 2,8,14,20-*para*-hydroxytetraphenylpyrogallol[4]arene as its hexa DMF solvate, (1).

The title compound (1) lies on an inversion center. The molecule exhibits a chair (rctt) conformation, characteristic of pyrogallol[4]arenes with aromatic substituents. In this molecule, the pyrogallol ring (C2A to C7A) is separated from its symmetry inverse ring (C2A^{vi} to C7A^{i}, symmetry code vi = $-x$, $1-y$, $1-z$) by a distance of 4.934 (2) Å, based on least squares mean planes of both rings. The other two pyrogallol rings (C2B to C7B and C2B^{vi} to C7B^{vi}) show an interplanar distance of 0.340 (2) Å. The dihedral angle between the pyrogallol rings not related by symmetry (C2A to C7A and C2B to C7B) is 83.64 (15)°, which indicates that the chair structure is slightly distorted from an ideal, right-angle chair conformation. Another interesting structural feature of this molecule is the position of the *p*-hydroxyphenyl substituents which are almost perfectly aligned one on top of the other, as in our previously reported compounds (Zambrano *et al.*, 2006). The centroid to centroid distance of the *p*-hydroxyphenyl rings (C8A to C13A and C8B to C13B) is 4.168 (2) Å, which suggests that there is no π-π interaction (Figure 1).

The asymmetric part of the unit cell contains three molecules of DMF, which are acting as hydrogen bond acceptors for a number the hydroxyl groups of the pyrogallolarene macrocycle and the OH group from the *p*-hydroxyphenyl substituents (Table 1). The hydrogen-bond distances are all unexceptional (Cave *et al.*, 2005), and these interactions contribute to the stability and molecular arrangement in the crystal packing (Figure 2).

Experimental

A 50 ml round bottom flask was charged with 2.0 g (16 mmol) pyrogallol and 11 ml 95% ethanol. The reaction vessel was cooled in an ice bath to 0 °C and 2.0 ml of concentrated HCl was added in one portion. *4*-hydroxybenzaldehyde (2.0 g, 17 mmol) was then added dropwise over a period of 10 minutes. The reaction vessel was allowed to warm slowly to room temperature and then maintained at 80 °C for 12 h, the pink precipitate that separated was collected by filtration and washed with cold 1:1 ethanol-water until the material was pale and neutral to pH paper. Drying under vacuum at 40 °C for 12 h afforded 10.3 g (28 mmol) of 2,8,14,20-*para*-hydroxytetra(phenyl)pyrogallol [4]arene, Yield, 70% mp >400 °C. Crystals suitable for X-ray diffraction were grown from a solution of the title compound in DMF by vapor diffusion of ether over a period of three days.

Refinement

Two solvate DMF molecules are flip-disordered by an approximate 180° rotation around the axis built by the oxygen and nitrogen atom. The occupancy ratios are 0.853 (2) to 0.147 (2) and 0.862 (2) to 0.138 (2), respectively. Atoms of the minor components were set to have the same anisotropic displacement parameters as their major component counterparts.

All hydrogen atoms were placed in calculated positions and were refined with an isotropic displacement parameter 1.5 (methyl, hydroxyl) or 1.2 times (all others) that of the adjacent carbon or oxygen atom. Methyl and hydroxyl H atoms were allowed to rotate to best fit the experimental electron density.

Figures

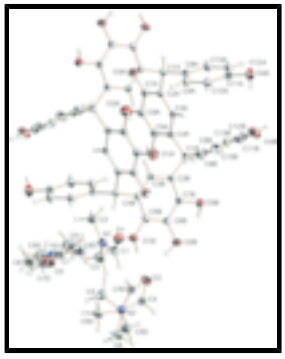

Fig. 1. Molecular structure of (1) Displacement ellipsoids are drawn at the 50% probability level. The labels of atoms of the minor disorder components of the two disordered DMF solvate molecules end with the letter D.

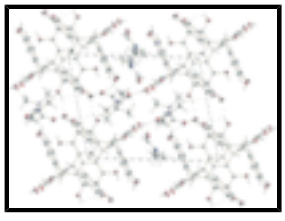

Fig. 2. Packing diagram of (1), viewed down the *a* axis. Dashed lines indicate hydrogen bonds. Atoms of the minor disorder components are omitted for clarity.

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Crystal data

$C_{52}H_{40}O_{16}\cdot 6C_3H_7NO$	$Z = 1$
$M_r = 1359.42$	$F_{000} = 720$
Triclinic, $P\overline{1}$	$D_x = 1.372$ Mg m^{-3}
$a = 10.6481$ (5) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 11.5153$ (6) Å	Cell parameters from 6320 reflections
$c = 14.3315$ (7) Å	$\theta = 2.5$–30.5º
$\alpha = 75.748$ (1)º	$\mu = 0.10$ mm^{-1}
$\beta = 78.462$ (1)º	$T = 100$ (2) K
$\gamma = 77.891$ (1)º	Rod, red
$V = 1644.8$ (1) Å^3	0.44 × 0.25 × 0.19 mm

Data collection

Bruker SMART APEX CCD diffractometer	8127 independent reflections
Radiation source: fine-focus sealed tube	7050 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.018$
$T = 100(2)$ K	$\theta_{max} = 28.3°$
ω scans	$\theta_{min} = 1.5°$
Absorption correction: multi-scan (SADABS in SAINT-Plus; Bruker, 2003)	$h = -14\rightarrow14$
$T_{min} = 0.914$, $T_{max} = 0.981$	$k = -15\rightarrow15$
17256 measured reflections	$l = -19\rightarrow18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.151$	$w = 1/[\sigma^2(F_o^2) + (0.0801P)^2 + 0.915P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
8127 reflections	$\Delta\rho_{max} = 0.61$ e Å^{-3}
472 parameters	$\Delta\rho_{min} = -0.30$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.99258 (17)	0.38850 (15)	0.28575 (12)	0.0307 (3)	
H1	0.9761	0.3275	0.3427	0.037*	
C2	0.99254 (17)	0.60148 (15)	0.21092 (12)	0.0312 (3)	
H2A	1.0539	0.5683	0.1594	0.047*	
H2B	1.0306	0.6599	0.2313	0.047*	

H2C	0.9116	0.6425	0.1862	0.047*	
C3	0.8999 (2)	0.53525 (18)	0.38644 (13)	0.0384 (4)	
H3A	0.8920	0.4611	0.4368	0.058*	
H3B	0.8131	0.5821	0.3786	0.058*	
H3C	0.9511	0.5844	0.4058	0.058*	
C1A	0.34385 (13)	1.16631 (13)	−0.21626 (10)	0.0201 (3)	
H1A	0.2936	1.2428	−0.2507	0.024*	
C2A	0.30150 (13)	1.15892 (13)	−0.10722 (10)	0.0194 (3)	
C3A	0.27753 (13)	1.05079 (12)	−0.04233 (10)	0.0185 (3)	
H3AA	0.2871	0.9799	−0.0675	0.022*	
C4A	0.24032 (13)	1.04211 (12)	0.05747 (10)	0.0193 (3)	
C5A	0.23045 (15)	1.14616 (13)	0.09418 (11)	0.0236 (3)	
C6A	0.25611 (16)	1.25525 (13)	0.03091 (12)	0.0256 (3)	
C7A	0.28926 (14)	1.26157 (13)	−0.06914 (11)	0.0225 (3)	
C8A	0.31036 (14)	1.06105 (13)	−0.24771 (10)	0.0213 (3)	
C9A	0.39940 (15)	0.95642 (14)	−0.25773 (11)	0.0252 (3)	
H9AA	0.4855	0.9499	−0.2457	0.030*	
C10A	0.36493 (16)	0.86066 (15)	−0.28505 (12)	0.0290 (3)	
H10A	0.4269	0.7894	−0.2914	0.035*	
C11A	0.23889 (16)	0.87018 (16)	−0.30292 (12)	0.0293 (3)	
C12A	0.14689 (15)	0.97112 (17)	−0.28887 (12)	0.0301 (3)	
H12A	0.0599	0.9758	−0.2980	0.036*	
C13A	0.18252 (15)	1.06538 (15)	−0.26145 (11)	0.0259 (3)	
H13A	0.1189	1.1345	−0.2517	0.031*	
C1B	0.20447 (13)	0.92516 (12)	0.12616 (10)	0.0183 (3)	
H1BA	0.1150	0.9462	0.1621	0.022*	
C2B	0.29434 (13)	0.87096 (12)	0.20181 (10)	0.0185 (3)	
C3B	0.42568 (13)	0.87979 (12)	0.18023 (10)	0.0193 (3)	
H3BA	0.4574	0.9261	0.1187	0.023*	
C4B	0.51240 (13)	0.82355 (13)	0.24508 (10)	0.0198 (3)	
C5B	0.46533 (14)	0.75684 (14)	0.33598 (11)	0.0232 (3)	
C6B	0.33437 (15)	0.74490 (14)	0.35918 (10)	0.0237 (3)	
C7B	0.24947 (14)	0.80255 (13)	0.29214 (10)	0.0211 (3)	
C8B	0.19900 (14)	0.83211 (12)	0.06797 (10)	0.0199 (3)	
C9B	0.30959 (16)	0.75285 (14)	0.03820 (12)	0.0273 (3)	
H9BA	0.3888	0.7511	0.0599	0.033*	
C10B	0.30687 (18)	0.67616 (15)	−0.02249 (13)	0.0343 (4)	
H10B	0.3832	0.6224	−0.0417	0.041*	
C11B	0.1916 (2)	0.67914 (14)	−0.05453 (12)	0.0329 (4)	
C12B	0.08049 (17)	0.75720 (15)	−0.02619 (12)	0.0308 (3)	
H12B	0.0016	0.7592	−0.0484	0.037*	
C13B	0.08468 (15)	0.83274 (14)	0.03490 (11)	0.0253 (3)	
H13B	0.0080	0.8858	0.0544	0.030*	
O2	0.42629 (13)	0.61912 (13)	0.59274 (9)	0.0381 (3)	0.862 (2)
N2	0.57745 (14)	0.54857 (13)	0.69391 (10)	0.0295 (3)	0.862 (2)
C4	0.46452 (18)	0.55243 (16)	0.66588 (13)	0.0269 (4)	0.862 (2)
H4A	0.4090	0.4989	0.7060	0.032*	0.862 (2)
C5	0.6704 (2)	0.6228 (3)	0.63664 (19)	0.0496 (6)	0.862 (2)
H5A	0.6324	0.6787	0.5821	0.074*	0.862 (2)

H5B	0.7486	0.5707	0.6114	0.074*	0.862 (2)
H5C	0.6937	0.6694	0.6774	0.074*	0.862 (2)
C6	0.6104 (2)	0.46902 (19)	0.78485 (15)	0.0345 (4)	0.862 (2)
H6A	0.5418	0.4202	0.8145	0.052*	0.862 (2)
H6B	0.6183	0.5182	0.8296	0.052*	0.862 (2)
H6C	0.6932	0.4151	0.7716	0.052*	0.862 (2)
O2D	0.42629 (13)	0.61912 (13)	0.59274 (9)	0.0381 (3)	0.138 (2)
N2D	0.57745 (14)	0.54857 (13)	0.69391 (10)	0.0295 (3)	0.138 (2)
C4D	0.5417 (12)	0.5776 (10)	0.6090 (9)	0.0269 (4)	0.138 (2)
H4DA	0.6069	0.5670	0.5545	0.032*	0.138 (2)
C5D	0.5114 (15)	0.5265 (17)	0.7842 (12)	0.0496 (6)	0.138 (2)
H5DA	0.4178	0.5478	0.7817	0.074*	0.138 (2)
H5DB	0.5349	0.5754	0.8231	0.074*	0.138 (2)
H5DC	0.5329	0.4401	0.8141	0.074*	0.138 (2)
C6D	0.7317 (13)	0.5371 (12)	0.6899 (10)	0.0345 (4)	0.138 (2)
H6DA	0.7763	0.5327	0.6238	0.052*	0.138 (2)
H6DB	0.7631	0.4632	0.7358	0.052*	0.138 (2)
H6DC	0.7494	0.6082	0.7078	0.052*	0.138 (2)
O3	0.96416 (13)	0.75896 (13)	0.49257 (9)	0.0406 (3)	0.853 (2)
N3	0.79212 (15)	0.90216 (15)	0.53217 (11)	0.0371 (3)	0.853 (2)
C7	0.85173 (19)	0.81247 (19)	0.48894 (13)	0.0308 (4)	0.853 (2)
H7	0.8032	0.7866	0.4513	0.037*	0.853 (2)
C8	0.8588 (3)	0.9613 (2)	0.58079 (18)	0.0502 (6)	0.853 (2)
H8A	0.9448	0.9129	0.5892	0.075*	0.853 (2)
H8B	0.8081	0.9687	0.6448	0.075*	0.853 (2)
H8C	0.8688	1.0424	0.5414	0.075*	0.853 (2)
C9	0.6571 (2)	0.9574 (3)	0.5217 (2)	0.0562 (7)	0.853 (2)
H9A	0.6524	1.0446	0.4938	0.084*	0.853 (2)
H9B	0.6024	0.9454	0.5858	0.084*	0.853 (2)
H9C	0.6264	0.9191	0.4785	0.084*	0.853 (2)
O3D	0.96416 (13)	0.75896 (13)	0.49257 (9)	0.0406 (3)	0.147 (2)
N3D	0.79212 (15)	0.90216 (15)	0.53217 (11)	0.0371 (3)	0.147 (2)
C7D	0.9189 (11)	0.8283 (11)	0.5317 (8)	0.0308 (4)	0.147 (2)
H7D	0.9706	0.8438	0.5727	0.037*	0.147 (2)
C8D	0.6903 (18)	0.8547 (14)	0.5047 (10)	0.0502 (6)	0.147 (2)
H8DA	0.7294	0.7831	0.4771	0.075*	0.147 (2)
H8DB	0.6470	0.9175	0.4561	0.075*	0.147 (2)
H8DC	0.6264	0.8320	0.5625	0.075*	0.147 (2)
C9D	0.7601 (15)	0.9996 (16)	0.5765 (12)	0.0562 (7)	0.147 (2)
H9DA	0.8377	1.0356	0.5707	0.084*	0.147 (2)
H9DB	0.7261	0.9723	0.6455	0.084*	0.147 (2)
H9DC	0.6936	1.0604	0.5449	0.084*	0.147 (2)
N1	0.96491 (13)	0.50275 (12)	0.29420 (10)	0.0270 (3)	
O1	1.03927 (14)	0.35553 (11)	0.20722 (9)	0.0385 (3)	
O1A	0.19421 (13)	1.13827 (10)	0.19257 (8)	0.0329 (3)	
H1AC	0.1457	1.2031	0.2027	0.049*	
O2A	0.25105 (14)	1.36112 (10)	0.06166 (9)	0.0355 (3)	
H2AA	0.1883	1.3681	0.1071	0.053*	
O3A	0.31120 (12)	1.36937 (10)	−0.13166 (8)	0.0281 (2)	

H3AB	0.2624	1.4275	−0.1101	0.042*
O4A	0.20173 (13)	0.78266 (13)	−0.33659 (10)	0.0398 (3)
H4AA	0.2328	0.7135	−0.3067	0.060*
O1B	0.55232 (11)	0.70030 (12)	0.39992 (8)	0.0332 (3)
H1BB	0.5112	0.6779	0.4558	0.050*
O2B	0.28093 (12)	0.67351 (12)	0.44388 (8)	0.0347 (3)
H2BA	0.3294	0.6603	0.4863	0.052*
O3B	0.12134 (10)	0.78879 (11)	0.31362 (8)	0.0270 (2)
H3BB	0.0963	0.7814	0.3739	0.041*
O4B	0.19297 (16)	0.60331 (12)	−0.11610 (11)	0.0466 (4)
H4BB	0.1199	0.6163	−0.1340	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0415 (9)	0.0288 (8)	0.0254 (7)	−0.0126 (7)	−0.0070 (6)	−0.0052 (6)
C2	0.0360 (9)	0.0252 (7)	0.0307 (8)	−0.0053 (6)	−0.0042 (6)	−0.0035 (6)
C3	0.0432 (10)	0.0424 (10)	0.0304 (9)	−0.0062 (8)	−0.0005 (7)	−0.0143 (8)
C1A	0.0194 (6)	0.0204 (6)	0.0205 (6)	−0.0040 (5)	−0.0056 (5)	−0.0019 (5)
C2A	0.0172 (6)	0.0209 (6)	0.0206 (6)	−0.0027 (5)	−0.0052 (5)	−0.0039 (5)
C3A	0.0167 (6)	0.0176 (6)	0.0223 (6)	−0.0015 (5)	−0.0055 (5)	−0.0053 (5)
C4A	0.0178 (6)	0.0178 (6)	0.0225 (7)	−0.0009 (5)	−0.0061 (5)	−0.0040 (5)
C5A	0.0278 (7)	0.0216 (7)	0.0220 (7)	−0.0012 (5)	−0.0065 (5)	−0.0062 (5)
C6A	0.0319 (8)	0.0197 (7)	0.0280 (7)	−0.0033 (6)	−0.0085 (6)	−0.0083 (6)
C7A	0.0230 (7)	0.0189 (6)	0.0261 (7)	−0.0039 (5)	−0.0066 (5)	−0.0032 (5)
C8A	0.0215 (7)	0.0260 (7)	0.0174 (6)	−0.0068 (5)	−0.0040 (5)	−0.0034 (5)
C9A	0.0232 (7)	0.0286 (7)	0.0266 (7)	−0.0060 (6)	−0.0064 (6)	−0.0076 (6)
C10A	0.0294 (8)	0.0294 (8)	0.0313 (8)	−0.0053 (6)	−0.0050 (6)	−0.0116 (6)
C11A	0.0319 (8)	0.0356 (8)	0.0261 (7)	−0.0140 (7)	−0.0024 (6)	−0.0118 (6)
C12A	0.0225 (7)	0.0438 (9)	0.0292 (8)	−0.0106 (6)	−0.0033 (6)	−0.0139 (7)
C13A	0.0215 (7)	0.0340 (8)	0.0238 (7)	−0.0052 (6)	−0.0034 (5)	−0.0087 (6)
C1B	0.0171 (6)	0.0188 (6)	0.0190 (6)	−0.0014 (5)	−0.0036 (5)	−0.0049 (5)
C2B	0.0198 (6)	0.0179 (6)	0.0187 (6)	−0.0023 (5)	−0.0042 (5)	−0.0051 (5)
C3B	0.0215 (6)	0.0179 (6)	0.0186 (6)	−0.0040 (5)	−0.0041 (5)	−0.0025 (5)
C4B	0.0189 (6)	0.0201 (6)	0.0215 (6)	−0.0046 (5)	−0.0047 (5)	−0.0040 (5)
C5B	0.0243 (7)	0.0250 (7)	0.0208 (7)	−0.0044 (5)	−0.0081 (5)	−0.0023 (5)
C6B	0.0255 (7)	0.0282 (7)	0.0172 (6)	−0.0081 (6)	−0.0034 (5)	−0.0012 (5)
C7B	0.0205 (6)	0.0244 (7)	0.0195 (6)	−0.0054 (5)	−0.0024 (5)	−0.0061 (5)
C8B	0.0241 (7)	0.0170 (6)	0.0188 (6)	−0.0046 (5)	−0.0054 (5)	−0.0019 (5)
C9B	0.0297 (8)	0.0257 (7)	0.0284 (8)	0.0027 (6)	−0.0117 (6)	−0.0096 (6)
C10B	0.0429 (10)	0.0270 (8)	0.0341 (9)	0.0094 (7)	−0.0164 (7)	−0.0135 (7)
C11B	0.0555 (11)	0.0200 (7)	0.0276 (8)	−0.0038 (7)	−0.0199 (7)	−0.0046 (6)
C12B	0.0366 (9)	0.0281 (8)	0.0323 (8)	−0.0105 (6)	−0.0152 (7)	−0.0029 (6)
C13B	0.0241 (7)	0.0248 (7)	0.0275 (7)	−0.0056 (6)	−0.0062 (6)	−0.0038 (6)
O2	0.0399 (7)	0.0472 (7)	0.0287 (6)	−0.0062 (6)	−0.0114 (5)	−0.0072 (5)
N2	0.0339 (7)	0.0274 (7)	0.0256 (7)	−0.0041 (5)	−0.0073 (5)	−0.0015 (5)
C4	0.0315 (9)	0.0239 (8)	0.0256 (8)	−0.0048 (7)	−0.0059 (7)	−0.0048 (7)
C5	0.0383 (12)	0.0636 (16)	0.0439 (13)	−0.0232 (11)	−0.0095 (10)	0.0092 (11)

C6	0.0394 (11)	0.0323 (10)	0.0311 (10)	−0.0034 (8)	−0.0144 (8)	−0.0005 (8)
O2D	0.0399 (7)	0.0472 (7)	0.0287 (6)	−0.0062 (6)	−0.0114 (5)	−0.0072 (5)
N2D	0.0339 (7)	0.0274 (7)	0.0256 (7)	−0.0041 (5)	−0.0073 (5)	−0.0015 (5)
C4D	0.0315 (9)	0.0239 (8)	0.0256 (8)	−0.0048 (7)	−0.0059 (7)	−0.0048 (7)
C5D	0.0383 (12)	0.0636 (16)	0.0439 (13)	−0.0232 (11)	−0.0095 (10)	0.0092 (11)
C6D	0.0394 (11)	0.0323 (10)	0.0311 (10)	−0.0034 (8)	−0.0144 (8)	−0.0005 (8)
O3	0.0375 (7)	0.0518 (8)	0.0267 (6)	0.0025 (6)	−0.0026 (5)	−0.0080 (6)
N3	0.0381 (8)	0.0426 (8)	0.0258 (7)	−0.0014 (7)	0.0001 (6)	−0.0071 (6)
C7	0.0320 (10)	0.0377 (10)	0.0201 (8)	−0.0069 (8)	−0.0019 (7)	−0.0022 (7)
C8	0.0756 (19)	0.0436 (13)	0.0323 (11)	−0.0084 (12)	−0.0094 (11)	−0.0104 (10)
C9	0.0368 (12)	0.0651 (17)	0.0442 (13)	0.0104 (11)	0.0074 (10)	0.0029 (12)
O3D	0.0375 (7)	0.0518 (8)	0.0267 (6)	0.0025 (6)	−0.0026 (5)	−0.0080 (6)
N3D	0.0381 (8)	0.0426 (8)	0.0258 (7)	−0.0014 (7)	0.0001 (6)	−0.0071 (6)
C7D	0.0320 (10)	0.0377 (10)	0.0201 (8)	−0.0069 (8)	−0.0019 (7)	−0.0022 (7)
C8D	0.0756 (19)	0.0436 (13)	0.0323 (11)	−0.0084 (12)	−0.0094 (11)	−0.0104 (10)
C9D	0.0368 (12)	0.0651 (17)	0.0442 (13)	0.0104 (11)	0.0074 (10)	0.0029 (12)
N1	0.0316 (7)	0.0275 (6)	0.0238 (6)	−0.0081 (5)	−0.0037 (5)	−0.0068 (5)
O1	0.0587 (8)	0.0298 (6)	0.0296 (6)	−0.0093 (6)	−0.0064 (6)	−0.0101 (5)
O1A	0.0539 (8)	0.0221 (5)	0.0219 (5)	−0.0017 (5)	−0.0061 (5)	−0.0072 (4)
O2A	0.0559 (8)	0.0219 (5)	0.0320 (6)	−0.0101 (5)	−0.0051 (5)	−0.0103 (5)
O3A	0.0371 (6)	0.0188 (5)	0.0278 (6)	−0.0067 (4)	−0.0046 (5)	−0.0028 (4)
O4A	0.0379 (7)	0.0434 (7)	0.0486 (8)	−0.0140 (6)	−0.0073 (6)	−0.0229 (6)
O1B	0.0267 (6)	0.0477 (7)	0.0216 (5)	−0.0097 (5)	−0.0090 (4)	0.0066 (5)
O2B	0.0306 (6)	0.0508 (7)	0.0198 (5)	−0.0151 (5)	−0.0059 (4)	0.0065 (5)
O3B	0.0204 (5)	0.0380 (6)	0.0215 (5)	−0.0086 (4)	−0.0008 (4)	−0.0031 (4)
O4B	0.0759 (10)	0.0280 (6)	0.0459 (8)	0.0043 (6)	−0.0357 (7)	−0.0164 (6)

Geometric parameters (Å, °)

C1—O1	1.251 (2)	C9B—C10B	1.391 (2)
C1—N1	1.317 (2)	C9B—H9BA	0.9500
C1—H1	0.9500	C10B—C11B	1.385 (3)
C2—N1	1.461 (2)	C10B—H10B	0.9500
C2—H2A	0.9800	C11B—O4B	1.3822 (19)
C2—H2B	0.9800	C11B—C12B	1.384 (3)
C2—H2C	0.9800	C12B—C13B	1.390 (2)
C3—N1	1.461 (2)	C12B—H12B	0.9500
C3—H3A	0.9800	C13B—H13B	0.9500
C3—H3B	0.9800	O2—C4	1.224 (2)
C3—H3C	0.9800	N2—C4	1.331 (2)
C1A—C8A	1.5212 (19)	N2—C5	1.438 (3)
C1A—C2A	1.5236 (19)	N2—C6	1.456 (2)
C1A—C4B^{i}	1.5249 (19)	C4—H4A	0.9500
C1A—H1A	1.0000	C5—H5A	0.9800
C2A—C7A	1.392 (2)	C5—H5B	0.9800
C2A—C3A	1.3959 (19)	C5—H5C	0.9800
C3A—C4A	1.390 (2)	C6—H6A	0.9800
C3A—H3AA	0.9500	C6—H6B	0.9800
C4A—C5A	1.400 (2)	C6—H6C	0.9800

C4A—C1B	1.5300 (19)	C4D—H4DA	0.9500
C5A—O1A	1.3710 (18)	C5D—H5DA	0.9800
C5A—C6A	1.400 (2)	C5D—H5DB	0.9800
C6A—O2A	1.3823 (18)	C5D—H5DC	0.9800
C6A—C7A	1.394 (2)	C6D—H6DA	0.9800
C7A—O3A	1.3742 (18)	C6D—H6DB	0.9800
C8A—C9A	1.387 (2)	C6D—H6DC	0.9800
C8A—C13A	1.403 (2)	O3—C7	1.231 (2)
C9A—C10A	1.394 (2)	N3—C7	1.318 (3)
C9A—H9AA	0.9500	N3—C8	1.445 (3)
C10A—C11A	1.393 (2)	N3—C9	1.466 (3)
C10A—H10A	0.9500	C7—H7	0.9500
C11A—O4A	1.3742 (19)	C8—H8A	0.9800
C11A—C12A	1.382 (2)	C8—H8B	0.9800
C12A—C13A	1.385 (2)	C8—H8C	0.9800
C12A—H12A	0.9500	C9—H9A	0.9800
C13A—H13A	0.9500	C9—H9B	0.9800
C1B—C2B	1.5205 (18)	C9—H9C	0.9800
C1B—C8B	1.5273 (19)	C7D—H7D	0.9500
C1B—H1BA	1.0000	C8D—H8DA	0.9800
C2B—C3B	1.3903 (19)	C8D—H8DB	0.9800
C2B—C7B	1.3904 (19)	C8D—H8DC	0.9800
C3B—C4B	1.3900 (19)	C9D—H9DA	0.9800
C3B—H3BA	0.9500	C9D—H9DB	0.9800
C4B—C5B	1.395 (2)	C9D—H9DC	0.9800
C4B—C1A^{i}	1.5249 (19)	O1A—H1AC	0.8400
C5B—O1B	1.3836 (17)	O2A—H2AA	0.8400
C5B—C6B	1.395 (2)	O3A—H3AB	0.8400
C6B—O2B	1.3791 (18)	O4A—H4AA	0.8400
C6B—C7B	1.401 (2)	O1B—H1BB	0.8400
C7B—O3B	1.3711 (17)	O2B—H2BA	0.8400
C8B—C13B	1.390 (2)	O3B—H3BB	0.8400
C8B—C9B	1.393 (2)	O4B—H4BB	0.8400
O1—C1—N1	123.91 (16)	C3B—C2B—C1B	121.21 (12)
O1—C1—H1	118.0	C7B—C2B—C1B	120.64 (12)
N1—C1—H1	118.0	C4B—C3B—C2B	122.67 (13)
N1—C2—H2A	109.5	C4B—C3B—H3BA	118.7
N1—C2—H2B	109.5	C2B—C3B—H3BA	118.7
H2A—C2—H2B	109.5	C3B—C4B—C5B	118.62 (13)
N1—C2—H2C	109.5	C3B—C4B—C1A^{i}	120.30 (12)
H2A—C2—H2C	109.5	C5B—C4B—C1A^{i}	121.08 (12)
H2B—C2—H2C	109.5	O1B—C5B—C4B	118.34 (13)
N1—C3—H3A	109.5	O1B—C5B—C6B	121.62 (13)
N1—C3—H3B	109.5	C4B—C5B—C6B	120.00 (13)
H3A—C3—H3B	109.5	O2B—C6B—C5B	124.23 (13)
N1—C3—H3C	109.5	O2B—C6B—C7B	115.71 (13)
H3A—C3—H3C	109.5	C5B—C6B—C7B	119.98 (13)
H3B—C3—H3C	109.5	O3B—C7B—C2B	118.98 (13)

C8A—C1A—C2A	111.44 (11)	O3B—C7B—C6B	120.22 (13)
C8A—C1A—C4B^{i}	112.76 (12)	C2B—C7B—C6B	120.76 (13)
C2A—C1A—C4B^{i}	110.53 (11)	C13B—C8B—C9B	117.86 (13)
C8A—C1A—H1A	107.3	C13B—C8B—C1B	120.08 (13)
C2A—C1A—H1A	107.3	C9B—C8B—C1B	121.76 (13)
C4B^{i}—C1A—H1A	107.3	C10B—C9B—C8B	121.61 (15)
C7A—C2A—C3A	117.90 (13)	C10B—C9B—H9BA	119.2
C7A—C2A—C1A	119.84 (13)	C8B—C9B—H9BA	119.2
C3A—C2A—C1A	122.23 (12)	C11B—C10B—C9B	119.20 (16)
C4A—C3A—C2A	122.99 (13)	C11B—C10B—H10B	120.4
C4A—C3A—H3AA	118.5	C9B—C10B—H10B	120.4
C2A—C3A—H3AA	118.5	O4B—C11B—C12B	121.99 (16)
C3A—C4A—C5A	118.02 (13)	O4B—C11B—C10B	117.68 (16)
C3A—C4A—C1B	122.04 (12)	C12B—C11B—C10B	120.33 (15)
C5A—C4A—C1B	119.87 (13)	C11B—C12B—C13B	119.74 (15)
O1A—C5A—C4A	118.40 (13)	C11B—C12B—H12B	120.1
O1A—C5A—C6A	121.47 (13)	C13B—C12B—H12B	120.1
C4A—C5A—C6A	120.13 (13)	C8B—C13B—C12B	121.25 (15)
O2A—C6A—C7A	116.13 (13)	C8B—C13B—H13B	119.4
O2A—C6A—C5A	123.60 (14)	C12B—C13B—H13B	119.4
C7A—C6A—C5A	120.27 (13)	C4—N2—C5	121.66 (16)
O3A—C7A—C2A	118.98 (13)	C4—N2—C6	120.65 (16)
O3A—C7A—C6A	120.38 (13)	C5—N2—C6	117.69 (17)
C2A—C7A—C6A	120.64 (13)	O2—C4—N2	125.45 (17)
C9A—C8A—C13A	117.89 (14)	O2—C4—H4A	117.3
C9A—C8A—C1A	122.63 (13)	N2—C4—H4A	117.3
C13A—C8A—C1A	119.36 (13)	H5DA—C5D—H5DB	109.5
C8A—C9A—C10A	121.21 (14)	H5DA—C5D—H5DC	109.5
C8A—C9A—H9AA	119.4	H5DB—C5D—H5DC	109.5
C10A—C9A—H9AA	119.4	H6DA—C6D—H6DB	109.5
C11A—C10A—C9A	119.51 (15)	H6DA—C6D—H6DC	109.5
C11A—C10A—H10A	120.2	H6DB—C6D—H6DC	109.5
C9A—C10A—H10A	120.2	C7—N3—C8	122.68 (19)
O4A—C11A—C12A	117.60 (15)	C7—N3—C9	120.5 (2)
O4A—C11A—C10A	122.16 (15)	C8—N3—C9	116.4 (2)
C12A—C11A—C10A	120.23 (15)	O3—C7—N3	126.36 (19)
C11A—C12A—C13A	119.51 (14)	O3—C7—H7	116.8
C11A—C12A—H12A	120.2	N3—C7—H7	116.8
C13A—C12A—H12A	120.2	C1—N1—C3	120.86 (15)
C12A—C13A—C8A	121.50 (15)	C1—N1—C2	121.32 (14)
C12A—C13A—H13A	119.2	C3—N1—C2	117.76 (14)
C8A—C13A—H13A	119.2	C5A—O1A—H1AC	109.5
C2B—C1B—C8B	110.91 (11)	C6A—O2A—H2AA	109.5
C2B—C1B—C4A	113.22 (11)	C7A—O3A—H3AB	109.5
C8B—C1B—C4A	110.42 (11)	C11A—O4A—H4AA	109.5
C2B—C1B—H1BA	107.3	C5B—O1B—H1BB	109.5
C8B—C1B—H1BA	107.3	C6B—O2B—H2BA	109.5
C4A—C1B—H1BA	107.3	C7B—O3B—H3BB	109.5

C3B—C2B—C7B	117.95 (13)	C11B—O4B—H4BB	109.5
C8A—C1A—C2A—C7A	−161.80 (13)	C4A—C1B—C2B—C3B	−33.95 (17)
C4B^{i}—C1A—C2A—C7A	71.99 (16)	C8B—C1B—C2B—C7B	−83.93 (16)
C8A—C1A—C2A—C3A	20.07 (18)	C4A—C1B—C2B—C7B	151.29 (13)
C4B^{i}—C1A—C2A—C3A	−106.15 (14)	C7B—C2B—C3B—C4B	−0.1 (2)
C7A—C2A—C3A—C4A	1.1 (2)	C1B—C2B—C3B—C4B	−175.04 (13)
C1A—C2A—C3A—C4A	179.23 (12)	C2B—C3B—C4B—C5B	−0.8 (2)
C2A—C3A—C4A—C5A	−1.9 (2)	C2B—C3B—C4B—C1A^{i}	178.35 (12)
C2A—C3A—C4A—C1B	175.21 (12)	C3B—C4B—C5B—O1B	179.51 (13)
C3A—C4A—C5A—O1A	−179.80 (13)	C1A^{i}—C4B—C5B—O1B	0.3 (2)
C1B—C4A—C5A—O1A	3.0 (2)	C3B—C4B—C5B—C6B	1.7 (2)
C3A—C4A—C5A—C6A	0.8 (2)	C1A^{i}—C4B—C5B—C6B	−177.45 (13)
C1B—C4A—C5A—C6A	−176.43 (13)	O1B—C5B—C6B—O2B	−2.8 (2)
O1A—C5A—C6A—O2A	2.0 (2)	C4B—C5B—C6B—O2B	174.88 (15)
C4A—C5A—C6A—O2A	−178.65 (14)	O1B—C5B—C6B—C7B	−179.36 (14)
O1A—C5A—C6A—C7A	−178.21 (14)	C4B—C5B—C6B—C7B	−1.7 (2)
C4A—C5A—C6A—C7A	1.2 (2)	C3B—C2B—C7B—O3B	−177.59 (12)
C3A—C2A—C7A—O3A	−179.41 (12)	C1B—C2B—C7B—O3B	−2.7 (2)
C1A—C2A—C7A—O3A	2.4 (2)	C3B—C2B—C7B—C6B	0.2 (2)
C3A—C2A—C7A—C6A	1.0 (2)	C1B—C2B—C7B—C6B	175.17 (13)
C1A—C2A—C7A—C6A	−177.21 (13)	O2B—C6B—C7B—O3B	1.6 (2)
O2A—C6A—C7A—O3A	−1.8 (2)	C5B—C6B—C7B—O3B	178.46 (13)
C5A—C6A—C7A—O3A	178.30 (13)	O2B—C6B—C7B—C2B	−176.17 (13)
O2A—C6A—C7A—C2A	177.73 (13)	C5B—C6B—C7B—C2B	0.7 (2)
C5A—C6A—C7A—C2A	−2.1 (2)	C2B—C1B—C8B—C13B	146.49 (13)
C2A—C1A—C8A—C9A	−96.49 (16)	C4A—C1B—C8B—C13B	−87.17 (15)
C4B^{i}—C1A—C8A—C9A	28.49 (19)	C2B—C1B—C8B—C9B	−39.95 (18)
C2A—C1A—C8A—C13A	79.36 (16)	C4A—C1B—C8B—C9B	86.39 (16)
C4B^{i}—C1A—C8A—C13A	−155.66 (13)	C13B—C8B—C9B—C10B	−0.1 (2)
C13A—C8A—C9A—C10A	3.0 (2)	C1B—C8B—C9B—C10B	−173.84 (15)
C1A—C8A—C9A—C10A	178.86 (14)	C8B—C9B—C10B—C11B	0.4 (3)
C8A—C9A—C10A—C11A	0.2 (2)	C9B—C10B—C11B—O4B	178.88 (16)
C9A—C10A—C11A—O4A	175.37 (15)	C9B—C10B—C11B—C12B	−0.2 (3)
C9A—C10A—C11A—C12A	−3.3 (3)	O4B—C11B—C12B—C13B	−179.19 (16)
O4A—C11A—C12A—C13A	−175.59 (15)	C10B—C11B—C12B—C13B	−0.1 (3)
C10A—C11A—C12A—C13A	3.1 (3)	C9B—C8B—C13B—C12B	−0.2 (2)
C11A—C12A—C13A—C8A	0.1 (2)	C1B—C8B—C13B—C12B	173.59 (14)
C9A—C8A—C13A—C12A	−3.1 (2)	C11B—C12B—C13B—C8B	0.4 (2)
C1A—C8A—C13A—C12A	−179.18 (14)	C5—N2—C4—O2	−2.2 (3)
C3A—C4A—C1B—C2B	117.68 (14)	C6—N2—C4—O2	177.31 (18)
C5A—C4A—C1B—C2B	−65.21 (16)	C8—N3—C7—O3	8.4 (3)
C3A—C4A—C1B—C8B	−7.35 (18)	C9—N3—C7—O3	−179.8 (2)
C5A—C4A—C1B—C8B	169.75 (13)	O1—C1—N1—C3	174.55 (17)
C8B—C1B—C2B—C3B	90.82 (15)	O1—C1—N1—C2	−2.6 (3)

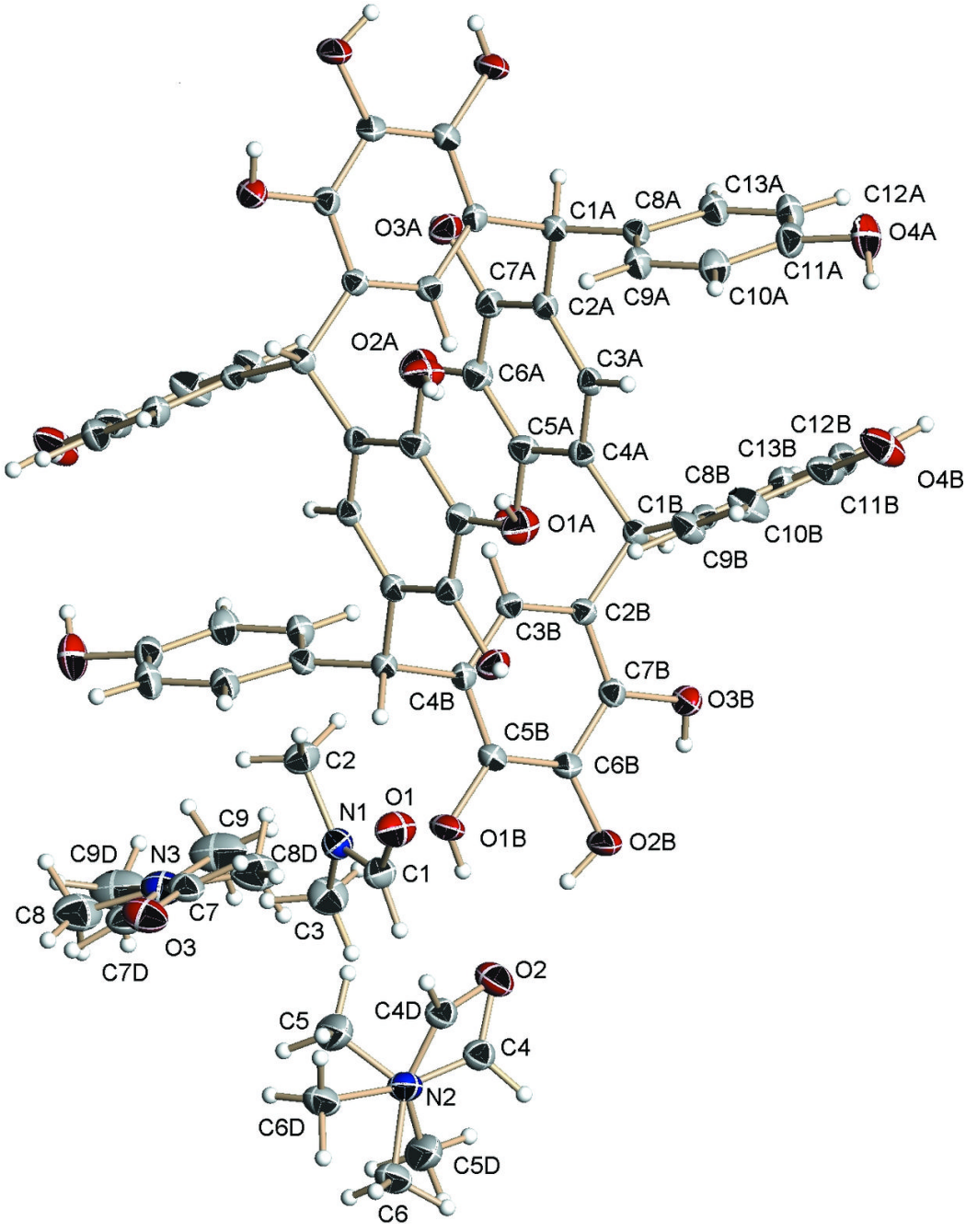
Symmetry codes: (i) −*x*+1, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4B—H4BB···O1^{ii}	0.84	2.10	2.923 (2)	168
O3B—H3BB···O3D^{iii}	0.84	1.98	2.7545 (17)	153
O3B—H3BB···O3^{iii}	0.84	1.98	2.7545 (17)	153
O2B—H2BA···O2D	0.84	1.92	2.7561 (17)	174
O2B—H2BA···O2	0.84	1.92	2.7561 (17)	174
O1B—H1BB···O2D	0.84	2.00	2.8429 (17)	176
O1B—H1BB···O2	0.84	2.00	2.8429 (17)	176
O4A—H4AA···O2D^{iv}	0.84	2.48	2.8933 (19)	111
O4A—H4AA···O2^{iv}	0.84	2.48	2.8933 (19)	111
O3A—H3AB···O4B^{v}	0.84	1.99	2.7663 (17)	153
O2A—H2AA···O1^{vi}	0.84	1.92	2.7484 (19)	169
O1A—H1AC···O1^{vi}	0.84	1.89	2.7227 (18)	172

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*; (iii) *x*−1, *y*, *z*; (iv) *x*, *y*, *z*−1; (v) *x*, *y*+1, *z*; (vi) *x*−1, *y*+1, *z*.

Fig. 1


C13A
C12A
C1A
C8A
O3A
O4A
C7A
C11A
C9A
C10A
C2A
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C6A
C3A
C5A
C12B
C4A
C13B
C8B
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O1
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C9
O1B
O2B
C9D
N3
C8D
C1
C8
C7
C3
O3
C7D
O2
C4D
C5
C4
N2
C6D
C5D
C6

Fig. 2