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Estradiol methanol hemisolvate

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Abstract

Initiation and progress of the majority of breast cancer cases are influenced by a family of hormones called estrogens. Estradiol is one of the three naturally occurring estrogens. This submission reports estradiol in a previously unknown crystal modification as methanol hemisolvate.

Refinement

Data collection was performed at three different 2theta settings and 0.15* increments in omega corresponding to more than one nominal sphere of data. Frame time was set at 16 s for the low angle measurements, 32 s for the medium setting, and 64 s for the high angle measurements. The decay correction was applied simultaneously with the absorption correction in *SADABS*. The final unit cell is obtained from the refinement of the XYZ weighted centroids of reflections above 20 σ(I).

Computing details

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997b); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

(sad)

Crystal data

$C_{18}H_{24}O_2 \cdot 0.5CH_4O$	γ = 70.7680 (3)°
M_r = 288.39	V = 793.080 (6) Å^3
Triclinic, $P\overline{1}$	Z = 2
a = 7.2989 (1) Å	Mo $K\alpha$
b = 9.2859 (1) Å	μ = 0.08 mm^{-1}
c = 12.4017 (1) Å	T = 100 (1) K
α = 89.4709 (3)°	0.42 × 0.26 × 0.22 mm
β = 87.8567 (2)°	

Data collection

Bruker Platform with 1K Area Detector diffractometer	47428 independent reflections
Absorption correction: empirical (using intensity measurements) multipole expansion (Blessing, 1995)	28997 reflections with $I > 2\sigma(I)$

T_{min} = 0.854, T_{max} = 1.000
90739 measured reflections

R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.116
S = 0.94
47428 reflections
587 parameters
3 restraints

All H-atom parameters refined
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter: 0.0 (2)

Table 1
Selected geometric parameters (Å, °)

C8B—C14B	1.5251 (6)	C9A—C11A	1.5397 (6)
C8B—C7B	1.5280 (6)	C9A—C8A	1.5471 (6)
C8B—C9B	1.5451 (6)	C9A—H9A	0.980 (12)
C8B—H8B	0.934 (12)	C8A—C14A	1.5243 (6)
C9B—C10B	1.5271 (6)	C8A—C7A	1.5277 (6)
C9B—C11B	1.5426 (6)	C8A—H8A	0.966 (12)
C9B—H9B	0.995 (12)	O1A—C3A	1.3726 (5)
C10B—C1B	1.4038 (6)	O1A—H1AA	0.809 (13)
C10B—C5B	1.4097 (6)	C5A—C4A	1.4000 (6)
C14B—C15B	1.5366 (7)	C5A—C6A	1.5144 (6)
C14B—C13B	1.5421 (6)	C4A—C3A	1.3922 (6)
C14B—H14B	0.974 (12)	C4A—H4A	0.990 (13)
C5B—C4B	1.4010 (6)	C3A—C2A	1.3959 (7)
C5B—C6B	1.5157 (6)	C14A—C15A	1.5425 (7)
C13B—C12B	1.5335 (7)	C14A—C13A	1.5432 (6)
C13B—C18B	1.5339 (7)	C14A—H14A	0.974 (12)
C13B—C17B	1.5431 (6)	C13A—C12A	1.5295 (6)
C4B—C3B	1.3946 (7)	C13A—C18A	1.5374 (7)
C4B—H4B	0.953 (11)	C13A—C17A	1.5390 (6)
C7B—C6B	1.5273 (7)	C1A—C2A	1.3948 (6)
C7B—H7C	0.998 (13)	C1A—H1A	0.950 (12)
C7B—H7D	0.955 (13)	O2A—C17A	1.4300 (6)
C12B—C11B	1.5415 (7)	O2A—H2AA	0.823 (15)
C12B—H12C	0.968 (14)	C11A—C12A	1.5405 (7)
C12B—H12D	0.955 (12)	C11A—H11A	0.993 (11)
O1B—C3B	1.3716 (6)	C11A—H11B	1.053 (13)
O1B—H1BB	0.810 (13)	C6A—C7A	1.5278 (7)
C1B—C2B	1.3946 (7)	C6A—H6B	1.040 (13)
C1B—H1B	0.979 (11)	C6A—H6A	1.004 (11)
C3B—C2B	1.3940 (7)	C2A—H2A	0.954 (12)
O2B—C17B	1.4314 (6)	C7A—H7A	0.968 (13)
O2B—H2BB	0.785 (13)	C7A—H7B	0.979 (14)
C11B—H11D	0.965 (17)	C12A—H12B	0.955 (12)

C11B—H11C	0.979 (14)	C12A—H12A	1.000 (14)
C6B—H6D	0.991 (12)	C17A—C16A	1.5461 (8)
C6B—H6C	0.930 (12)	C17A—H17A	0.976 (13)
C17B—C16B	1.5520 (8)	C18A—H18A	0.961 (11)
C17B—H17B	0.948 (12)	C18A—H18B	0.936 (13)
C2B—H2B	0.954 (13)	C18A—H18C	0.937 (14)
C18B—H18E	1.005 (14)	C16A—C15A	1.5560 (8)
C18B—H18D	0.933 (14)	C16A—H16A	0.999 (14)
C18B—H18F	0.900 (14)	C16A—H16B	1.005 (14)
C15B—C16B	1.5507 (8)	C15A—H15A	1.041 (14)
C15B—H15C	0.984 (15)	C15A—H15B	0.963 (15)
C15B—H15D	1.013 (16)	O3—C19	1.4261 (10)
C16B—H16C	1.030 (14)	O3—H3AA	0.719 (16)
C16B—H16D	0.995 (14)	C19—H19A	0.922 (17)
C10A—C1A	1.4024 (6)	C19—H19B	0.904 (16)
C10A—C5A	1.4071 (6)	C19—H19C	0.962 (19)
C10A—C9A	1.5244 (6)		
C14B—C8B—C7B	112.87 (4)	C10A—C9A—C8A	112.04 (3)
C14B—C8B—C9B	108.69 (3)	C11A—C9A—C8A	111.33 (3)
C7B—C8B—C9B	108.74 (4)	C10A—C9A—H9A	106.1 (7)
C14B—C8B—H8B	109.6 (8)	C11A—C9A—H9A	106.1 (7)
C7B—C8B—H8B	108.5 (8)	C8A—C9A—H9A	105.9 (7)
C9B—C8B—H8B	108.4 (7)	C14A—C8A—C7A	112.35 (4)
C10B—C9B—C11B	114.21 (4)	C14A—C8A—C9A	107.61 (3)
C10B—C9B—C8B	111.27 (3)	C7A—C8A—C9A	109.26 (4)
C11B—C9B—C8B	111.89 (4)	C14A—C8A—H8A	109.5 (7)
C10B—C9B—H9B	107.4 (7)	C7A—C8A—H8A	107.4 (7)
C11B—C9B—H9B	106.9 (7)	C9A—C8A—H8A	110.8 (7)
C8B—C9B—H9B	104.6 (7)	C3A—O1A—H1AA	107.1 (9)
C1B—C10B—C5B	117.55 (4)	C4A—C5A—C10A	120.00 (4)
C1B—C10B—C9B	121.51 (4)	C4A—C5A—C6A	118.46 (4)
C5B—C10B—C9B	120.88 (4)	C10A—C5A—C6A	121.50 (4)
C8B—C14B—C15B	119.62 (4)	C3A—C4A—C5A	121.19 (4)
C8B—C14B—C13B	113.35 (4)	C3A—C4A—H4A	119.6 (7)
C15B—C14B—C13B	103.72 (4)	C5A—C4A—H4A	119.2 (8)
C8B—C14B—H14B	107.7 (7)	O1A—C3A—C4A	117.98 (4)
C15B—C14B—H14B	107.9 (7)	O1A—C3A—C2A	122.51 (4)
C13B—C14B—H14B	103.3 (7)	C4A—C3A—C2A	119.52 (4)
C4B—C5B—C10B	120.29 (4)	C8A—C14A—C15A	120.19 (4)
C4B—C5B—C6B	117.78 (4)	C8A—C14A—C13A	113.48 (4)
C10B—C5B—C6B	121.91 (4)	C15A—C14A—C13A	103.89 (4)
C12B—C13B—C18B	110.13 (5)	C8A—C14A—H14A	104.5 (6)
C12B—C13B—C14B	108.37 (4)	C15A—C14A—H14A	107.5 (6)
C18B—C13B—C14B	113.51 (4)	C13A—C14A—H14A	106.5 (7)
C12B—C13B—C17B	115.62 (4)	C12A—C13A—C18A	110.13 (4)
C18B—C13B—C17B	109.56 (4)	C12A—C13A—C17A	115.10 (4)
C14B—C13B—C17B	99.37 (4)	C18A—C13A—C17A	110.67 (4)
C3B—C4B—C5B	120.94 (4)	C12A—C13A—C14A	109.03 (4)
C3B—C4B—H4B	120.3 (7)	C18A—C13A—C14A	113.64 (4)

C5B—C4B—H4B	118.8 (7)	C17A—C13A—C14A	97.86 (4)
C6B—C7B—C8B	110.21 (4)	C2A—C1A—C10A	122.42 (4)
C6B—C7B—H7C	111.1 (7)	C2A—C1A—H1A	114.8 (7)
C8B—C7B—H7C	107.7 (7)	C10A—C1A—H1A	122.8 (7)
C6B—C7B—H7D	110.3 (8)	C17A—O2A—H2AA	108.2 (10)
C8B—C7B—H7D	112.4 (8)	C9A—C11A—C12A	111.98 (4)
H7C—C7B—H7D	105.0 (11)	C9A—C11A—H11A	109.9 (6)
C13B—C12B—C11B	111.12 (4)	C12A—C11A—H11A	110.2 (6)
C13B—C12B—H12C	113.3 (8)	C9A—C11A—H11B	108.3 (7)
C11B—C12B—H12C	109.4 (8)	C12A—C11A—H11B	110.2 (7)
C13B—C12B—H12D	109.2 (7)	H11A—C11A—H11B	106.1 (9)
C11B—C12B—H12D	109.2 (7)	C5A—C6A—C7A	113.29 (4)
H12C—C12B—H12D	104.3 (11)	C5A—C6A—H6B	111.8 (7)
C3B—O1B—H1BB	113.4 (9)	C7A—C6A—H6B	112.3 (7)
C2B—C1B—C10B	122.30 (4)	C5A—C6A—H6A	107.3 (6)
C2B—C1B—H1B	116.6 (7)	C7A—C6A—H6A	108.6 (6)
C10B—C1B—H1B	121.1 (7)	H6B—C6A—H6A	102.9 (9)
O1B—C3B—C2B	118.38 (4)	C1A—C2A—C3A	119.05 (4)
O1B—C3B—C4B	122.09 (4)	C1A—C2A—H2A	121.8 (8)
C2B—C3B—C4B	119.53 (4)	C3A—C2A—H2A	119.2 (7)
C17B—O2B—H2BB	111.5 (9)	C8A—C7A—C6A	110.49 (4)
C12B—C11B—C9B	112.23 (4)	C8A—C7A—H7A	106.5 (8)
C12B—C11B—H11D	104.0 (10)	C6A—C7A—H7A	110.0 (7)
C9B—C11B—H11D	112.1 (10)	C8A—C7A—H7B	112.4 (8)
C12B—C11B—H11C	110.7 (8)	C6A—C7A—H7B	106.1 (8)
C9B—C11B—H11C	109.1 (8)	H7A—C7A—H7B	111.4 (11)
H11D—C11B—H11C	108.6 (13)	C13A—C12A—C11A	111.41 (4)
C5B—C6B—C7B	113.61 (4)	C13A—C12A—H12B	109.9 (7)
C5B—C6B—H6D	107.6 (7)	C11A—C12A—H12B	107.1 (7)
C7B—C6B—H6D	110.3 (7)	C13A—C12A—H12A	109.6 (8)
C5B—C6B—H6C	108.3 (7)	C11A—C12A—H12A	109.6 (8)
C7B—C6B—H6C	108.1 (7)	H12B—C12A—H12A	109.1 (11)
H6D—C6B—H6C	108.8 (10)	O2A—C17A—C13A	117.01 (4)
O2B—C17B—C13B	115.65 (4)	O2A—C17A—C16A	114.71 (4)
O2B—C17B—C16B	112.88 (4)	C13A—C17A—C16A	104.39 (4)
C13B—C17B—C16B	104.64 (4)	O2A—C17A—H17A	104.7 (8)
O2B—C17B—H17B	104.2 (8)	C13A—C17A—H17A	105.5 (7)
C13B—C17B—H17B	110.3 (8)	C16A—C17A—H17A	110.2 (7)
C16B—C17B—H17B	109.1 (7)	C13A—C18A—H18A	112.4 (7)
C3B—C2B—C1B	119.39 (5)	C13A—C18A—H18B	110.5 (8)
C3B—C2B—H2B	119.4 (8)	H18A—C18A—H18B	105.3 (10)
C1B—C2B—H2B	121.2 (8)	C13A—C18A—H18C	114.7 (9)
C13B—C18B—H18E	107.5 (8)	H18A—C18A—H18C	107.4 (11)
C13B—C18B—H18D	111.9 (9)	H18B—C18A—H18C	105.8 (12)
H18E—C18B—H18D	107.6 (12)	C17A—C16A—C15A	105.18 (4)
C13B—C18B—H18F	110.1 (10)	C17A—C16A—H16A	110.3 (8)
H18E—C18B—H18F	108.2 (12)	C15A—C16A—H16A	110.5 (8)
H18D—C18B—H18F	111.3 (13)	C17A—C16A—H16B	110.3 (9)
C14B—C15B—C16B	103.54 (5)	C15A—C16A—H16B	114.7 (8)

C14B—C15B—H15C	110.7 (8)	H16A—C16A—H16B	105.9 (11)
C16B—C15B—H15C	110.8 (9)	C14A—C15A—C16A	103.48 (4)
C14B—C15B—H15D	110.5 (8)	C14A—C15A—H15A	110.8 (7)
C16B—C15B—H15D	113.6 (9)	C16A—C15A—H15A	111.7 (7)
H15C—C15B—H15D	107.6 (12)	C14A—C15A—H15B	107.7 (9)
C15B—C16B—C17B	105.98 (4)	C16A—C15A—H15B	114.6 (9)
C15B—C16B—H16C	112.4 (8)	H15A—C15A—H15B	108.5 (11)
C17B—C16B—H16C	109.4 (7)	C19—O3—H3AA	112.4 (13)
C15B—C16B—H16D	110.7 (8)	O3—C19—H19A	108.7 (11)
C17B—C16B—H16D	111.2 (8)	O3—C19—H19B	107.1 (11)
H16C—C16B—H16D	107.2 (11)	H19A—C19—H19B	110.5 (15)
C1A—C10A—C5A	117.70 (4)	O3—C19—H19C	111.4 (11)
C1A—C10A—C9A	121.17 (4)	H19A—C19—H19C	110.9 (15)
C5A—C10A—C9A	120.95 (4)	H19B—C19—H19C	108.2 (15)
C10A—C9A—C11A	114.59 (4)		

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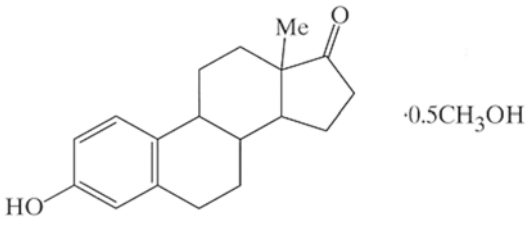
CIF access

Scheme 1



supplementary materials

(sad)

Crystal data

$C_{18}H_{24}O_2 \cdot 0.5CH_4O$	$Z = 2$
$M_r = 288.39$	$F_{000} = 314$
Triclinic, $P\overline{1}$	$D_x = 1.208$ Mg m^{-3}
$a = 7.2989$ (1) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 9.2859$ (1) Å	Cell parameters from 24302 reflections
$c = 12.4017$ (1) Å	$\theta = 1.6$–71.6º
$\alpha = 89.4709$ (3)º	$\mu = 0.08$ mm^{-1}
$\beta = 87.8567$ (2)º	$T = 100$ (1) K
$\gamma = 70.7680$ (3)º	Clear prism, colorless
$V = 793.080$ (6) Å^3	0.42 × 0.26 × 0.22 mm

Data collection

Bruker Platform with 1K Area Detector diffractometer	47428 independent reflections
Radiation source: fine-focus sealed tube	28997 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.039$
$T = 100(1)$ K	$\theta_{max} = 71.6$º
ω scans	$\theta_{min} = 1.6$º
Absorption correction: empirical (using intensity measurements) multipole expansion (Blessing, 1995)	$h = -19 \rightarrow 18$
$T_{min} = 0.854$, $T_{max} = 1.000$	$k = -24 \rightarrow 22$
90739 measured reflections	$l = -31 \rightarrow 33$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.055P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.116$	$(\Delta/\sigma)_{max} = 0.003$
$S = 0.94$	$\Delta\rho_{max} = 0.49$ e Å^{-3}
47428 reflections	$\Delta\rho_{min} = -0.28$ e Å^{-3}
587 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983)
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.0 (2)
Secondary atom site location: difference Fourier map	

Special details

Experimental. Data collection was performed at three different 2theta settings and 0.15* increments in omega corresponding to more than one nominal sphere of data. Frame time was set at 16 s for the low angle measurements, 32 s for the medium setting, and 64 s for the high angle measurements. The decay correction was applied simultaneously with the absorption correction in *SADABS* (Sheldrick, 1996). The final unit cell is obtained from the refinement of the XYZ weighted centroids of reflections above 20 σ(I).

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C8B	0.04166 (6)	0.24672 (5)	0.66125 (3)	0.01395 (5)
C9B	0.24572 (6)	0.13501 (5)	0.63045 (3)	0.01482 (5)
C10B	0.29189 (6)	0.14068 (5)	0.50968 (3)	0.01526 (6)
C14B	0.00026 (6)	0.22961 (5)	0.78128 (3)	0.01525 (6)
C5B	0.14195 (6)	0.19058 (5)	0.43571 (3)	0.01462 (5)
C13B	0.15031 (7)	0.26042 (5)	0.85392 (3)	0.01474 (5)
C4B	0.18627 (7)	0.18998 (5)	0.32479 (3)	0.01608 (6)
C7B	−0.10627 (7)	0.21365 (7)	0.59004 (4)	0.01825 (7)
C12B	0.35097 (7)	0.14616 (6)	0.82397 (4)	0.01865 (7)
O1B	0.42578 (7)	0.14065 (6)	0.17733 (3)	0.02324 (7)
C1B	0.48384 (7)	0.09030 (7)	0.46772 (4)	0.02074 (8)
C3B	0.37842 (7)	0.14070 (6)	0.28541 (4)	0.01753 (6)
O2B	0.13758 (7)	0.29192 (5)	1.05583 (3)	0.02172 (7)
C11B	0.40242 (7)	0.15571 (7)	0.70301 (4)	0.02056 (8)
C6B	−0.07016 (7)	0.24990 (7)	0.47238 (4)	0.01910 (7)
C17B	0.06340 (8)	0.23698 (6)	0.96541 (4)	0.01764 (6)
C2B	0.52846 (8)	0.08974 (7)	0.35736 (4)	0.02229 (9)
C18B	0.15539 (11)	0.42399 (6)	0.84564 (4)	0.02330 (9)
C15B	−0.19608 (8)	0.32562 (9)	0.83307 (5)	0.02588 (11)
C16B	−0.15908 (9)	0.31328 (9)	0.95567 (4)	0.02580 (10)
C10A	0.09402 (6)	0.73660 (5)	0.64247 (3)	0.01371 (5)
C9A	0.10870 (6)	0.67359 (5)	0.52823 (3)	0.01395 (5)
C8A	0.30044 (6)	0.66872 (5)	0.46833 (3)	0.01421 (5)
O1A	0.06268 (6)	0.85651 (5)	0.96969 (3)	0.01943 (6)
C5A	0.26187 (6)	0.72632 (5)	0.69859 (3)	0.01410 (5)
C4A	0.24640 (7)	0.76733 (5)	0.80775 (3)	0.01567 (6)
C3A	0.06640 (7)	0.82216 (5)	0.86205 (3)	0.01544 (6)
C14A	0.31055 (6)	0.58769 (5)	0.36084 (3)	0.01553 (6)

C13A	0.13926 (7)	0.66714 (5)	0.28826 (3)	0.01478 (5)
C1A	−0.08589 (6)	0.79587 (6)	0.69813 (4)	0.01676 (6)
O2A	0.08601 (7)	0.59357 (5)	0.09879 (3)	0.02049 (6)
C11A	−0.06816 (7)	0.75182 (6)	0.45963 (4)	0.01800 (7)
C6A	0.46088 (7)	0.67702 (6)	0.64264 (4)	0.01817 (7)
C2A	−0.10222 (7)	0.84035 (6)	0.80615 (4)	0.01758 (6)
C7A	0.47122 (7)	0.58731 (6)	0.53864 (4)	0.01841 (7)
C12A	−0.05088 (7)	0.67541 (6)	0.34826 (4)	0.01808 (7)
C17A	0.19830 (8)	0.55378 (6)	0.19324 (4)	0.01713 (6)
C18A	0.13279 (9)	0.82719 (6)	0.25135 (4)	0.02006 (7)
C16A	0.41795 (9)	0.52517 (7)	0.17383 (4)	0.02283 (9)
C15A	0.49109 (8)	0.55705 (8)	0.28445 (4)	0.02301 (9)
O3	0.69894 (8)	0.93820 (6)	0.04874 (5)	0.02844 (9)
C19	0.62122 (11)	0.81599 (10)	0.05404 (6)	0.02970 (12)
H6B	0.5693 (18)	0.6202 (15)	0.6949 (10)	0.028 (3)*
H7C	−0.0930 (18)	0.1039 (15)	0.5991 (10)	0.028 (3)*
H14A	0.2986 (16)	0.4893 (13)	0.3804 (9)	0.019 (2)*
H9A	0.1141 (17)	0.5672 (14)	0.5359 (10)	0.022 (2)*
H12B	−0.1587 (17)	0.7354 (14)	0.3082 (10)	0.023 (2)*
H9B	0.2369 (17)	0.0322 (14)	0.6463 (10)	0.023 (3)*
H6D	−0.1425 (17)	0.2050 (13)	0.4242 (9)	0.023 (2)*
H12A	−0.0580 (19)	0.5702 (15)	0.3574 (11)	0.032 (3)*
H6C	−0.1148 (17)	0.3554 (14)	0.4643 (10)	0.025 (3)*
H1B	0.5938 (16)	0.0552 (13)	0.5154 (9)	0.019 (2)*
H15C	−0.232 (2)	0.4323 (17)	0.8090 (12)	0.039 (3)*
H16C	−0.2300 (19)	0.2479 (15)	0.9953 (11)	0.034 (3)*
H8B	0.0410 (17)	0.3459 (14)	0.6474 (10)	0.024 (3)*
H7A	0.4607 (18)	0.4882 (14)	0.5553 (10)	0.027 (3)*
H15A	0.5380 (19)	0.6515 (15)	0.2809 (11)	0.031 (3)*
H18A	0.1114 (16)	0.8976 (13)	0.3106 (9)	0.021 (2)*
H12C	0.454 (2)	0.1584 (16)	0.8663 (11)	0.035 (3)*
H4A	0.3654 (18)	0.7612 (15)	0.8459 (11)	0.028 (3)*
H6A	0.4926 (15)	0.7720 (12)	0.6245 (8)	0.015 (2)*
H17A	0.1767 (18)	0.4612 (15)	0.2197 (10)	0.027 (3)*
H2A	−0.2254 (18)	0.8820 (14)	0.8430 (10)	0.027 (3)*
H7B	0.5966 (19)	0.5782 (16)	0.5031 (11)	0.033 (3)*
H2B	0.6598 (18)	0.0547 (15)	0.3302 (10)	0.030 (3)*
H11A	−0.1891 (16)	0.7513 (12)	0.4988 (9)	0.018 (2)*
H18E	0.259 (2)	0.4318 (16)	0.8938 (11)	0.037 (3)*
H14B	0.0169 (17)	0.1226 (13)	0.7947 (9)	0.022 (2)*
H7D	−0.2370 (18)	0.2684 (15)	0.6129 (10)	0.029 (3)*
H11D	0.526 (2)	0.075 (2)	0.6924 (14)	0.054 (4)*
H19A	0.687 (2)	0.743 (2)	0.0035 (14)	0.051 (4)*
H17B	0.0912 (17)	0.1315 (14)	0.9794 (10)	0.025 (3)*
H1A	−0.2055 (17)	0.8054 (13)	0.6662 (9)	0.022 (2)*
H11C	0.421 (2)	0.2535 (16)	0.6864 (11)	0.035 (3)*
H16A	0.4394 (19)	0.5964 (15)	0.1177 (11)	0.033 (3)*
H18D	0.187 (2)	0.4475 (16)	0.7757 (11)	0.035 (3)*
H15B	0.593 (2)	0.4723 (17)	0.3132 (12)	0.037 (3)*

H2BB	0.1091 (18)	0.3812 (15)	1.0551 (10)	0.028 (3)*
H11B	−0.0798 (17)	0.8673 (14)	0.4505 (10)	0.026 (3)*
H4B	0.0825 (16)	0.2245 (13)	0.2763 (9)	0.021 (2)*
H18F	0.041 (2)	0.4905 (17)	0.8697 (12)	0.038 (3)*
H18B	0.0287 (19)	0.8696 (15)	0.2062 (11)	0.033 (3)*
H16B	0.484 (2)	0.4195 (16)	0.1444 (12)	0.040 (4)*
H1AA	−0.0502 (19)	0.8929 (14)	0.9891 (11)	0.028 (3)*
H18C	0.244 (2)	0.8303 (17)	0.2122 (11)	0.036 (3)*
H16D	−0.205 (2)	0.4159 (16)	0.9901 (12)	0.037 (3)*
H8A	0.3037 (16)	0.7706 (14)	0.4554 (9)	0.020 (2)*
H12D	0.3513 (17)	0.0453 (14)	0.8402 (10)	0.024 (3)*
H15D	−0.302 (2)	0.2851 (17)	0.8115 (12)	0.043 (4)*
H1BB	0.3353 (18)	0.1882 (15)	0.1414 (10)	0.029 (3)*
H19B	0.494 (2)	0.8555 (19)	0.0388 (13)	0.046 (4)*
H2AA	0.111 (2)	0.6650 (17)	0.0690 (12)	0.037 (3)*
H19C	0.630 (3)	0.773 (2)	0.1252 (15)	0.059 (5)*
H3AA	0.650 (2)	0.9987 (19)	0.0859 (13)	0.047 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C8B	0.01313 (12)	0.01481 (13)	0.01331 (11)	−0.00376 (10)	−0.00104 (9)	0.00126 (10)
C9B	0.01345 (13)	0.01578 (14)	0.01356 (12)	−0.00238 (11)	−0.00233 (10)	0.00020 (10)
C10B	0.01319 (13)	0.01694 (15)	0.01367 (12)	−0.00220 (11)	−0.00125 (10)	−0.00097 (10)
C14B	0.01557 (14)	0.01739 (15)	0.01330 (12)	−0.00613 (12)	−0.00066 (10)	0.00105 (10)
C5B	0.01371 (13)	0.01573 (14)	0.01359 (11)	−0.00362 (11)	−0.00156 (10)	−0.00016 (10)
C13B	0.01835 (15)	0.01336 (13)	0.01321 (11)	−0.00608 (11)	−0.00170 (10)	0.00085 (9)
C4B	0.01598 (14)	0.01747 (15)	0.01355 (12)	−0.00373 (12)	−0.00122 (10)	−0.00109 (10)
C7B	0.01435 (14)	0.0265 (2)	0.01506 (13)	−0.00824 (14)	−0.00206 (11)	0.00231 (13)
C12B	0.01681 (15)	0.02285 (18)	0.01479 (13)	−0.00417 (13)	−0.00387 (11)	0.00035 (12)
O1B	0.02171 (16)	0.02867 (19)	0.01403 (11)	−0.00134 (13)	0.00218 (10)	−0.00291 (11)
C1B	0.01339 (14)	0.0279 (2)	0.01614 (14)	−0.00027 (14)	−0.00094 (11)	−0.00188 (14)
C3B	0.01721 (15)	0.01854 (16)	0.01415 (12)	−0.00234 (12)	0.00089 (11)	−0.00282 (11)
O2B	0.03252 (19)	0.01869 (14)	0.01380 (11)	−0.00782 (13)	−0.00464 (11)	−0.00037 (10)
C11B	0.01424 (15)	0.0313 (2)	0.01502 (14)	−0.00578 (15)	−0.00275 (11)	−0.00036 (14)
C6B	0.01342 (14)	0.0279 (2)	0.01458 (13)	−0.00487 (14)	−0.00189 (11)	0.00244 (13)
C17B	0.02332 (18)	0.01692 (15)	0.01329 (12)	−0.00744 (14)	−0.00096 (12)	0.00041 (11)
C2B	0.01514 (16)	0.0301 (2)	0.01673 (15)	−0.00084 (15)	0.00086 (12)	−0.00334 (15)
C18B	0.0382 (3)	0.01660 (17)	0.01854 (16)	−0.01353 (18)	−0.00270 (17)	0.00138 (13)
C15B	0.01710 (17)	0.0398 (3)	0.01654 (16)	−0.00387 (19)	0.00130 (13)	0.00009 (17)
C16B	0.0224 (2)	0.0369 (3)	0.01579 (15)	−0.0069 (2)	0.00257 (14)	−0.00101 (17)
C10A	0.01284 (12)	0.01589 (14)	0.01260 (11)	−0.00500 (10)	−0.00030 (9)	0.00047 (10)
C9A	0.01283 (12)	0.01648 (14)	0.01296 (11)	−0.00543 (11)	−0.00026 (9)	−0.00025 (10)
C8A	0.01229 (12)	0.01590 (14)	0.01399 (11)	−0.00406 (10)	0.00001 (9)	−0.00091 (10)
O1A	0.02463 (16)	0.02130 (15)	0.01294 (10)	−0.00843 (12)	0.00063 (10)	−0.00197 (9)
C5A	0.01321 (12)	0.01521 (14)	0.01372 (11)	−0.00439 (10)	−0.00130 (10)	0.00067 (10)
C4A	0.01717 (15)	0.01663 (14)	0.01392 (12)	−0.00639 (12)	−0.00184 (11)	0.00028 (10)
C3A	0.01904 (15)	0.01498 (14)	0.01295 (11)	−0.00655 (12)	−0.00004 (10)	0.00013 (10)

C14A	0.01476 (14)	0.01672 (15)	0.01436 (12)	−0.00429 (11)	0.00091 (10)	−0.00174 (10)
C13A	0.01691 (14)	0.01490 (13)	0.01293 (11)	−0.00582 (11)	0.00029 (10)	−0.00138 (10)
C1A	0.01347 (13)	0.02235 (18)	0.01430 (12)	−0.00577 (12)	0.00063 (10)	−0.00061 (12)
O2A	0.02951 (18)	0.01909 (14)	0.01382 (10)	−0.00906 (13)	−0.00277 (11)	−0.00071 (9)
C11A	0.01280 (13)	0.0256 (2)	0.01433 (13)	−0.00458 (13)	−0.00064 (10)	−0.00235 (12)
C6A	0.01215 (13)	0.02405 (19)	0.01704 (14)	−0.00406 (12)	−0.00193 (11)	−0.00112 (13)
C2A	0.01659 (15)	0.02150 (18)	0.01430 (13)	−0.00601 (13)	0.00169 (11)	−0.00084 (12)
C7A	0.01302 (13)	0.02073 (17)	0.01823 (15)	−0.00103 (12)	−0.00123 (11)	−0.00219 (13)
C12A	0.01590 (15)	0.0249 (2)	0.01474 (13)	−0.00837 (14)	−0.00090 (11)	−0.00196 (12)
C17A	0.02186 (17)	0.01617 (15)	0.01372 (12)	−0.00675 (13)	−0.00003 (12)	−0.00202 (11)
C18A	0.0285 (2)	0.01600 (15)	0.01633 (14)	−0.00816 (15)	−0.00054 (14)	−0.00014 (12)
C16A	0.0228 (2)	0.0273 (2)	0.01759 (16)	−0.00752 (17)	0.00495 (14)	−0.00646 (15)
C15A	0.01677 (17)	0.0317 (3)	0.01876 (17)	−0.00584 (16)	0.00357 (13)	−0.00579 (16)
O3	0.0283 (2)	0.0267 (2)	0.02850 (19)	−0.00794 (16)	0.01260 (16)	−0.00697 (15)
C19	0.0289 (3)	0.0341 (3)	0.0276 (2)	−0.0130 (2)	0.0040 (2)	0.0010 (2)

Geometric parameters (Å, °)

C8B—C14B	1.5251 (6)	C9A—C11A	1.5397 (6)
C8B—C7B	1.5280 (6)	C9A—C8A	1.5471 (6)
C8B—C9B	1.5451 (6)	C9A—H9A	0.980 (12)
C8B—H8B	0.934 (12)	C8A—C14A	1.5243 (6)
C9B—C10B	1.5271 (6)	C8A—C7A	1.5277 (6)
C9B—C11B	1.5426 (6)	C8A—H8A	0.966 (12)
C9B—H9B	0.995 (12)	O1A—C3A	1.3726 (5)
C10B—C1B	1.4038 (6)	O1A—H1AA	0.809 (13)
C10B—C5B	1.4097 (6)	C5A—C4A	1.4000 (6)
C14B—C15B	1.5366 (7)	C5A—C6A	1.5144 (6)
C14B—C13B	1.5421 (6)	C4A—C3A	1.3922 (6)
C14B—H14B	0.974 (12)	C4A—H4A	0.990 (13)
C5B—C4B	1.4010 (6)	C3A—C2A	1.3959 (7)
C5B—C6B	1.5157 (6)	C14A—C15A	1.5425 (7)
C13B—C12B	1.5335 (7)	C14A—C13A	1.5432 (6)
C13B—C18B	1.5339 (7)	C14A—H14A	0.974 (12)
C13B—C17B	1.5431 (6)	C13A—C12A	1.5295 (6)
C4B—C3B	1.3946 (7)	C13A—C18A	1.5374 (7)
C4B—H4B	0.953 (11)	C13A—C17A	1.5390 (6)
C7B—C6B	1.5273 (7)	C1A—C2A	1.3948 (6)
C7B—H7C	0.998 (13)	C1A—H1A	0.950 (12)
C7B—H7D	0.955 (13)	O2A—C17A	1.4300 (6)
C12B—C11B	1.5415 (7)	O2A—H2AA	0.823 (15)
C12B—H12C	0.968 (14)	C11A—C12A	1.5405 (7)
C12B—H12D	0.955 (12)	C11A—H11A	0.993 (11)
O1B—C3B	1.3716 (6)	C11A—H11B	1.053 (13)
O1B—H1BB	0.810 (13)	C6A—C7A	1.5278 (7)
C1B—C2B	1.3946 (7)	C6A—H6B	1.040 (13)
C1B—H1B	0.979 (11)	C6A—H6A	1.004 (11)
C3B—C2B	1.3940 (7)	C2A—H2A	0.954 (12)
O2B—C17B	1.4314 (6)	C7A—H7A	0.968 (13)

O2B—H2BB	0.785 (13)	C7A—H7B	0.979 (14)
C11B—H11D	0.965 (17)	C12A—H12B	0.955 (12)
C11B—H11C	0.979 (14)	C12A—H12A	1.000 (14)
C6B—H6D	0.991 (12)	C17A—C16A	1.5461 (8)
C6B—H6C	0.930 (12)	C17A—H17A	0.976 (13)
C17B—C16B	1.5520 (8)	C18A—H18A	0.961 (11)
C17B—H17B	0.948 (12)	C18A—H18B	0.936 (13)
C2B—H2B	0.954 (13)	C18A—H18C	0.937 (14)
C18B—H18E	1.005 (14)	C16A—C15A	1.5560 (8)
C18B—H18D	0.933 (14)	C16A—H16A	0.999 (14)
C18B—H18F	0.900 (14)	C16A—H16B	1.005 (14)
C15B—C16B	1.5507 (8)	C15A—H15A	1.041 (14)
C15B—H15C	0.984 (15)	C15A—H15B	0.963 (15)
C15B—H15D	1.013 (16)	O3—C19	1.4261 (10)
C16B—H16C	1.030 (14)	O3—H3AA	0.719 (16)
C16B—H16D	0.995 (14)	C19—H19A	0.922 (17)
C10A—C1A	1.4024 (6)	C19—H19B	0.904 (16)
C10A—C5A	1.4071 (6)	C19—H19C	0.962 (19)
C10A—C9A	1.5244 (6)		
C14B—C8B—C7B	112.87 (4)	C10A—C9A—C8A	112.04 (3)
C14B—C8B—C9B	108.69 (3)	C11A—C9A—C8A	111.33 (3)
C7B—C8B—C9B	108.74 (4)	C10A—C9A—H9A	106.1 (7)
C14B—C8B—H8B	109.6 (8)	C11A—C9A—H9A	106.1 (7)
C7B—C8B—H8B	108.5 (8)	C8A—C9A—H9A	105.9 (7)
C9B—C8B—H8B	108.4 (7)	C14A—C8A—C7A	112.35 (4)
C10B—C9B—C11B	114.21 (4)	C14A—C8A—C9A	107.61 (3)
C10B—C9B—C8B	111.27 (3)	C7A—C8A—C9A	109.26 (4)
C11B—C9B—C8B	111.89 (4)	C14A—C8A—H8A	109.5 (7)
C10B—C9B—H9B	107.4 (7)	C7A—C8A—H8A	107.4 (7)
C11B—C9B—H9B	106.9 (7)	C9A—C8A—H8A	110.8 (7)
C8B—C9B—H9B	104.6 (7)	C3A—O1A—H1AA	107.1 (9)
C1B—C10B—C5B	117.55 (4)	C4A—C5A—C10A	120.00 (4)
C1B—C10B—C9B	121.51 (4)	C4A—C5A—C6A	118.46 (4)
C5B—C10B—C9B	120.88 (4)	C10A—C5A—C6A	121.50 (4)
C8B—C14B—C15B	119.62 (4)	C3A—C4A—C5A	121.19 (4)
C8B—C14B—C13B	113.35 (4)	C3A—C4A—H4A	119.6 (7)
C15B—C14B—C13B	103.72 (4)	C5A—C4A—H4A	119.2 (8)
C8B—C14B—H14B	107.7 (7)	O1A—C3A—C4A	117.98 (4)
C15B—C14B—H14B	107.9 (7)	O1A—C3A—C2A	122.51 (4)
C13B—C14B—H14B	103.3 (7)	C4A—C3A—C2A	119.52 (4)
C4B—C5B—C10B	120.29 (4)	C8A—C14A—C15A	120.19 (4)
C4B—C5B—C6B	117.78 (4)	C8A—C14A—C13A	113.48 (4)
C10B—C5B—C6B	121.91 (4)	C15A—C14A—C13A	103.89 (4)
C12B—C13B—C18B	110.13 (5)	C8A—C14A—H14A	104.5 (6)
C12B—C13B—C14B	108.37 (4)	C15A—C14A—H14A	107.5 (6)
C18B—C13B—C14B	113.51 (4)	C13A—C14A—H14A	106.5 (7)
C12B—C13B—C17B	115.62 (4)	C12A—C13A—C18A	110.13 (4)
C18B—C13B—C17B	109.56 (4)	C12A—C13A—C17A	115.10 (4)
C14B—C13B—C17B	99.37 (4)	C18A—C13A—C17A	110.67 (4)

C3B—C4B—C5B	120.94 (4)	C12A—C13A—C14A	109.03 (4)
C3B—C4B—H4B	120.3 (7)	C18A—C13A—C14A	113.64 (4)
C5B—C4B—H4B	118.8 (7)	C17A—C13A—C14A	97.86 (4)
C6B—C7B—C8B	110.21 (4)	C2A—C1A—C10A	122.42 (4)
C6B—C7B—H7C	111.1 (7)	C2A—C1A—H1A	114.8 (7)
C8B—C7B—H7C	107.7 (7)	C10A—C1A—H1A	122.8 (7)
C6B—C7B—H7D	110.3 (8)	C17A—O2A—H2AA	108.2 (10)
C8B—C7B—H7D	112.4 (8)	C9A—C11A—C12A	111.98 (4)
H7C—C7B—H7D	105.0 (11)	C9A—C11A—H11A	109.9 (6)
C13B—C12B—C11B	111.12 (4)	C12A—C11A—H11A	110.2 (6)
C13B—C12B—H12C	113.3 (8)	C9A—C11A—H11B	108.3 (7)
C11B—C12B—H12C	109.4 (8)	C12A—C11A—H11B	110.2 (7)
C13B—C12B—H12D	109.2 (7)	H11A—C11A—H11B	106.1 (9)
C11B—C12B—H12D	109.2 (7)	C5A—C6A—C7A	113.29 (4)
H12C—C12B—H12D	104.3 (11)	C5A—C6A—H6B	111.8 (7)
C3B—O1B—H1BB	113.4 (9)	C7A—C6A—H6B	112.3 (7)
C2B—C1B—C10B	122.30 (4)	C5A—C6A—H6A	107.3 (6)
C2B—C1B—H1B	116.6 (7)	C7A—C6A—H6A	108.6 (6)
C10B—C1B—H1B	121.1 (7)	H6B—C6A—H6A	102.9 (9)
O1B—C3B—C2B	118.38 (4)	C1A—C2A—C3A	119.05 (4)
O1B—C3B—C4B	122.09 (4)	C1A—C2A—H2A	121.8 (8)
C2B—C3B—C4B	119.53 (4)	C3A—C2A—H2A	119.2 (7)
C17B—O2B—H2BB	111.5 (9)	C8A—C7A—C6A	110.49 (4)
C12B—C11B—C9B	112.23 (4)	C8A—C7A—H7A	106.5 (8)
C12B—C11B—H11D	104.0 (10)	C6A—C7A—H7A	110.0 (7)
C9B—C11B—H11D	112.1 (10)	C8A—C7A—H7B	112.4 (8)
C12B—C11B—H11C	110.7 (8)	C6A—C7A—H7B	106.1 (8)
C9B—C11B—H11C	109.1 (8)	H7A—C7A—H7B	111.4 (11)
H11D—C11B—H11C	108.6 (13)	C13A—C12A—C11A	111.41 (4)
C5B—C6B—C7B	113.61 (4)	C13A—C12A—H12B	109.9 (7)
C5B—C6B—H6D	107.6 (7)	C11A—C12A—H12B	107.1 (7)
C7B—C6B—H6D	110.3 (7)	C13A—C12A—H12A	109.6 (8)
C5B—C6B—H6C	108.3 (7)	C11A—C12A—H12A	109.6 (8)
C7B—C6B—H6C	108.1 (7)	H12B—C12A—H12A	109.1 (11)
H6D—C6B—H6C	108.8 (10)	O2A—C17A—C13A	117.01 (4)
O2B—C17B—C13B	115.65 (4)	O2A—C17A—C16A	114.71 (4)
O2B—C17B—C16B	112.88 (4)	C13A—C17A—C16A	104.39 (4)
C13B—C17B—C16B	104.64 (4)	O2A—C17A—H17A	104.7 (8)
O2B—C17B—H17B	104.2 (8)	C13A—C17A—H17A	105.5 (7)
C13B—C17B—H17B	110.3 (8)	C16A—C17A—H17A	110.2 (7)
C16B—C17B—H17B	109.1 (7)	C13A—C18A—H18A	112.4 (7)
C3B—C2B—C1B	119.39 (5)	C13A—C18A—H18B	110.5 (8)
C3B—C2B—H2B	119.4 (8)	H18A—C18A—H18B	105.3 (10)
C1B—C2B—H2B	121.2 (8)	C13A—C18A—H18C	114.7 (9)
C13B—C18B—H18E	107.5 (8)	H18A—C18A—H18C	107.4 (11)
C13B—C18B—H18D	111.9 (9)	H18B—C18A—H18C	105.8 (12)
H18E—C18B—H18D	107.6 (12)	C17A—C16A—C15A	105.18 (4)
C13B—C18B—H18F	110.1 (10)	C17A—C16A—H16A	110.3 (8)
H18E—C18B—H18F	108.2 (12)	C15A—C16A—H16A	110.5 (8)

H18D—C18B—H18F	111.3 (13)	C17A—C16A—H16B	110.3 (9)
C14B—C15B—C16B	103.54 (5)	C15A—C16A—H16B	114.7 (8)
C14B—C15B—H15C	110.7 (8)	H16A—C16A—H16B	105.9 (11)
C16B—C15B—H15C	110.8 (9)	C14A—C15A—C16A	103.48 (4)
C14B—C15B—H15D	110.5 (8)	C14A—C15A—H15A	110.8 (7)
C16B—C15B—H15D	113.6 (9)	C16A—C15A—H15A	111.7 (7)
H15C—C15B—H15D	107.6 (12)	C14A—C15A—H15B	107.7 (9)
C15B—C16B—C17B	105.98 (4)	C16A—C15A—H15B	114.6 (9)
C15B—C16B—H16C	112.4 (8)	H15A—C15A—H15B	108.5 (11)
C17B—C16B—H16C	109.4 (7)	C19—O3—H3AA	112.4 (13)
C15B—C16B—H16D	110.7 (8)	O3—C19—H19A	108.7 (11)
C17B—C16B—H16D	111.2 (8)	O3—C19—H19B	107.1 (11)
H16C—C16B—H16D	107.2 (11)	H19A—C19—H19B	110.5 (15)
C1A—C10A—C5A	117.70 (4)	O3—C19—H19C	111.4 (11)
C1A—C10A—C9A	121.17 (4)	H19A—C19—H19C	110.9 (15)
C5A—C10A—C9A	120.95 (4)	H19B—C19—H19C	108.2 (15)
C10A—C9A—C11A	114.59 (4)		