Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Pterodondiol

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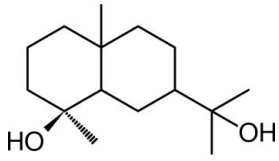
Received 2 February 2007; accepted 3 September 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.053; wR factor = 0.148; data-to-parameter ratio = 10.8.

The title compound, $C_{15}H_{28}O_2$, crystallizes with four molecules in the asymmetric unit. The molecules are linked by O—H···O and C—H···O intermolecular hydrogen bonds to form a continuous chain, which runs parallel to the a axis; intramolecular C—H···O hydrogen bonds are also present.

Related literature

For related literature, see: Jiangsu New Medical College (1977); Li & Ding (1993); Mei *et al.* (2006); Wei *et al.* (1995); Xiao *et al.* (2003); Flack (1983).



Experimental

Crystal data

$C_{15}H_{28}O_2$
M_r = 240.37
Monoclinic, $P2_1$
a = 15.9298 (16) Å
b = 11.8296 (12) Å
c = 16.8033 (17) Å
β = 108.502 (2)°
V = 3002.8 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.980, T_{max} = 0.993
25093 measured reflections
6858 independent reflections
4838 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.148
S = 1.05
6858 reflections
637 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O7^{i}	0.82	2.09	2.892 (3)	165
O5—H5A···O3^{ii}	0.82	2.04	2.815 (3)	158
O2—H2···O4	0.82	2.14	2.927 (3)	161
O3—H3···O2	0.82	2.04	2.851 (3)	171
O4—H4···O1	0.82	2.01	2.814 (3)	165
O6—H6···O8	0.82	1.98	2.782 (3)	166
O7—H7···O6	0.82	2.07	2.891 (3)	178
O8—H8···O5	0.82	1.93	2.719 (3)	160
C5—H5···O2	0.98	2.48	3.221 (3)	132
C5—H5···O4	0.98	2.59	3.422 (3)	143
C9—H9A···O2	0.97	2.59	3.201 (4)	121
C50—H50···O8	0.98	2.35	3.081 (4)	131
C20—H20···O4	0.98	2.44	3.163 (3)	130

Symmetry codes: (i) $x, y, z-1$; (ii) $-x+2, y-\frac{1}{2}, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

We are grateful to Dr Jian-chao Liu for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ER2031).

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  doi:10.1107/S1600536807043152

supplementary materials

Acta Cryst. (2007). E**63**, o4010 [**doi:10.1107/S1600536807043152**]

Pterodondiol

Z. Mei, Y. Li and G. Yang

Comment

Laggera pterodonta (DC) Benth (Compositae) has been used as traditional herbal medicine for its anti-inflammatory and anti-bacterial activities (Jiangsu New Medical College, 1977) in the South-West of China. Some eudesmane sesquiterpenes isolated from this plant showed cytotoxicity on tumor cells (Xiao *et al.*, 2003) and antibacterial activities (Wei *et al.*, 1995). These interesting activities on eudesmane sesquiterpenes have prompted us to isolate more sesquiterpenes to evaluate their biological activities. Earlier, we have reported the structure of pterodontic acid which was obtained from this plant (Mei *et al.*, 2006). Following our work, the structure of pterodondiol (I) (Li & Ding, 1993) is confirmed by X-ray analysis.

The molecular structure of (I) is shown in Fig. 1 and the molecular packing is shown in Fig. 2. The title compound crystallizes with four molecules in the asymmetric unit. These molecules are linked by O—H···O, C—H···O intermolecular hydrogen bonds and C—H···O intramolecular hydrogen bonds to form a continuous chain, which runs parallel to the *a* axis. The hydrogen bond of C5···O4 [3.422 (3) Å] is the longest among all the hydrogen bonds, as listed in the table 1.

Experimental

The air-dried aerial parts of the Laggera pterodonta (2 kg) was powered and extracted twice with water at 100 centigrade, 2 h each time. The water extracts was combined and concentrated to half of the original volume. Then it was partitioned with EtOAc and BuOH, respectively. The EtOAc and n-BuOH extracts were concentrated *in vacuo* to afford 20 g and 22 g of residue. The EtOAc portion was subjected to column chromgraphy over 200 g silica gel, using petrol ether/acetone gradients (from 9:1 to 0:1) as eluents. Combining the fractions with TLC (GF254) monitoring, eight fractions were obtained and compound (I) (2.0 g) was crystallized from the fraction 4 (3.5 g). ^{1}H-NMR (300 MHz, $CDCl_3$) δ: 1.27(s, H15), 1.26(s, H14), 1.08(s, H7), 0.89(s, H8). ^{13}C-NMR (125 MHz, $CDCl_3$) δ: 34.32(C1), 20.24(C2), 43.67(C3), 72.69(C4), 48.99(C5), 41.60(C6), 21.99(C7), 18.64(C8), 41.60(C9), 21.32(C10), 41.89(C11), 20.72(C12), 74.79(C13), 29.68(C14), 29.73(C15).

Refinement

The hydrogen atoms were geometrically placed and constrained to ride on the parent atom. The C—H bond distances are 0.96 Å for CH_3, 0.97 Å for CH_2, 0.98 Å for CH and 0.82 Å for the OH groups. The U_{iso}(H) = 1.5 U_{eq}(C,*O*) for the CH_3 and the OH groups. For all other H atoms U_{iso}(H) = 1.2 U_{eq}(C). The Flack (1983) parameter could not be reliable determined due to insufficient anomalous scattering effects from the title compound as it only contains C, H and O atoms. Thus the reflection data were merged.

Figures

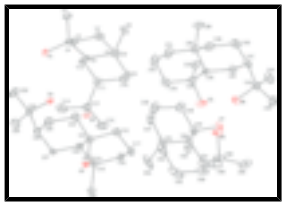

Fig. 1. The asymmetric unit, with atom labels and 50% probability displacement ellipsoids.

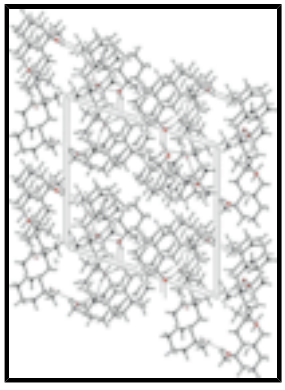

Fig. 2. The crystal packing, viewed along the *b* axis.

Pterodondiol

Crystal data

$C_{15}H_{28}O_2$	F_{000} = 1072
M_r = 240.37	D_x = 1.063 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 7823 reflections
a = 15.9298 (16) Å	θ = 2.2–22.1°
b = 11.8296 (12) Å	μ = 0.07 mm^{-1}
c = 16.8033 (17) Å	*T* = 298 (2) K
β = 108.502 (2)°	Block, colorless
V = 3002.8 (5) Å^3	0.30 × 0.20 × 0.10 mm
Z = 8	

Data collection

Bruker SMART 1K CCD diffractometer	6858 independent reflections
Radiation source: fine-focus sealed tube	4838 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
Detector resolution: 10 pixels mm^{-1}	θ_{max} = 27.0°
T = 298(2) K	θ_{min} = 1.3°
φ and ω scans	*h* = −20→20
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	*k* = −15→15

T_{min} = 0.980, T_{max} = 0.993
25093 measured reflections

l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.148
S = 1.05
6858 reflections
637 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0832P)^2 + 0.0769P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
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}
C1	0.6805 (3)	0.3024 (4)	0.2988 (2)	0.0806 (11)
H1A	0.6821	0.2445	0.3401	0.097*
H1B	0.7020	0.3720	0.3288	0.097*
C2	0.5859 (3)	0.3193 (4)	0.2443 (2)	0.0861 (11)
H2A	0.5507	0.3436	0.2789	0.103*
H2B	0.5620	0.2481	0.2183	0.103*
C3	0.5797 (2)	0.4065 (3)	0.1772 (2)	0.0708 (9)
H3A	0.5973	0.4794	0.2036	0.085*
H3B	0.5185	0.4124	0.1416	0.085*
C4	0.63714 (18)	0.3786 (3)	0.12292 (18)	0.0519 (7)
C5	0.73213 (17)	0.3553 (2)	0.17900 (16)	0.0446 (6)
H5	0.7513	0.4268	0.2086	0.053*
C6	0.7430 (2)	0.2680 (3)	0.25008 (19)	0.0621 (8)
C7	0.5957 (2)	0.2864 (4)	0.0592 (2)	0.0773 (10)

H7A	0.5399	0.3123	0.0221	0.116*
H7B	0.5866	0.2198	0.0881	0.116*
H7C	0.6346	0.2690	0.0274	0.116*
C8	0.7250 (3)	0.1439 (3)	0.2202 (3)	0.0982 (13)
H8A	0.7532	0.1286	0.1787	0.147*
H8B	0.6623	0.1323	0.1963	0.147*
H8C	0.7481	0.0940	0.2671	0.147*
C9	0.8393 (2)	0.2776 (3)	0.3068 (2)	0.0764 (10)
H9A	0.8483	0.3519	0.3325	0.092*
H9B	0.8496	0.2221	0.3515	0.092*
C10	0.9063 (2)	0.2598 (4)	0.2613 (3)	0.0874 (12)
H10A	0.9023	0.1821	0.2419	0.105*
H10B	0.9652	0.2706	0.3008	0.105*
C11	0.89499 (19)	0.3381 (3)	0.1865 (2)	0.0608 (8)
H11	0.9280	0.3023	0.1530	0.073*
C12	0.79764 (18)	0.3360 (3)	0.13096 (18)	0.0558 (7)
H12A	0.7887	0.3938	0.0881	0.067*
H12B	0.7852	0.2634	0.1028	0.067*
C13	0.93593 (18)	0.4575 (3)	0.2081 (2)	0.0611 (8)
C14	0.9266 (3)	0.5266 (4)	0.1300 (3)	0.1029 (14)
H14A	0.8649	0.5385	0.1003	0.154*
H14B	0.9535	0.4869	0.0946	0.154*
H14C	0.9553	0.5983	0.1456	0.154*
C15	1.0335 (2)	0.4493 (4)	0.2604 (3)	0.1044 (16)
H15A	1.0596	0.5232	0.2671	0.157*
H15B	1.0637	0.4010	0.2325	0.157*
H15C	1.0385	0.4184	0.3146	0.157*
C16	0.8048 (2)	0.5992 (3)	0.4825 (2)	0.0690 (9)
H16A	0.7688	0.5910	0.5191	0.083*
H16B	0.7925	0.5354	0.4443	0.083*
C17	0.9016 (2)	0.5968 (3)	0.5351 (2)	0.0717 (9)
H17A	0.9139	0.6579	0.5757	0.086*
H17B	0.9150	0.5260	0.5656	0.086*
C18	0.9593 (2)	0.6092 (3)	0.47947 (19)	0.0574 (7)
H18A	0.9511	0.5433	0.4434	0.069*
H18B	1.0208	0.6106	0.5146	0.069*
C19	0.94041 (17)	0.7153 (2)	0.42449 (16)	0.0476 (6)
C20	0.84052 (17)	0.7243 (2)	0.37757 (16)	0.0456 (6)
H20	0.8276	0.6592	0.3395	0.055*
C21	0.77886 (19)	0.7086 (3)	0.4319 (2)	0.0594 (7)
C22	0.9817 (2)	0.8201 (3)	0.4745 (2)	0.0705 (9)
H22A	1.0448	0.8113	0.4955	0.106*
H22B	0.9590	0.8296	0.5206	0.106*
H22C	0.9672	0.8854	0.4388	0.106*
C23	0.7795 (3)	0.8068 (4)	0.4923 (3)	0.0900 (12)
H23A	0.7298	0.7995	0.5126	0.135*
H23B	0.7757	0.8773	0.4631	0.135*
H23C	0.8334	0.8046	0.5388	0.135*
C24	0.6855 (2)	0.6953 (4)	0.3698 (3)	0.0812 (10)

H24A	0.6835	0.6275	0.3367	0.097*
H24B	0.6441	0.6854	0.4009	0.097*
C25	0.6566 (2)	0.7945 (4)	0.3115 (3)	0.0945 (13)
H25A	0.6514	0.8600	0.3443	0.113*
H25B	0.5982	0.7786	0.2727	0.113*
C26	0.7180 (2)	0.8245 (3)	0.2608 (2)	0.0716 (10)
H26	0.7040	0.9034	0.2437	0.086*
C27	0.8146 (2)	0.8267 (2)	0.3195 (2)	0.0621 (8)
H27A	0.8537	0.8308	0.2856	0.075*
H27B	0.8236	0.8947	0.3535	0.075*
C28	0.7042 (2)	0.7594 (3)	0.1781 (2)	0.0740 (10)
C29	0.6073 (3)	0.7624 (5)	0.1230 (3)	0.139 (2)
H29A	0.6005	0.7202	0.0725	0.208*
H29B	0.5896	0.8394	0.1089	0.208*
H29C	0.5710	0.7296	0.1529	0.208*
C30	0.7626 (4)	0.8073 (5)	0.1290 (3)	0.1244 (19)
H30A	0.8238	0.7966	0.1609	0.187*
H30B	0.7507	0.8866	0.1193	0.187*
H30C	0.7497	0.7688	0.0762	0.187*
C31	0.5705 (3)	0.2571 (5)	0.5550 (3)	0.0961 (14)
H31A	0.5696	0.3206	0.5912	0.115*
H31B	0.5098	0.2406	0.5218	0.115*
C32	0.6228 (3)	0.2903 (5)	0.4959 (3)	0.1102 (16)
H32A	0.6173	0.2311	0.4546	0.132*
H32B	0.5982	0.3592	0.4663	0.132*
C33	0.7199 (3)	0.3087 (4)	0.5443 (3)	0.0888 (12)
H33A	0.7252	0.3750	0.5795	0.107*
H33B	0.7513	0.3243	0.5046	0.107*
C34	0.76484 (19)	0.2101 (3)	0.59922 (19)	0.0596 (8)
C35	0.70828 (17)	0.1758 (2)	0.65495 (17)	0.0493 (6)
H35	0.7098	0.2418	0.6906	0.059*
C36	0.60917 (19)	0.1551 (3)	0.6090 (2)	0.0704 (9)
C37	0.7850 (2)	0.1154 (3)	0.5466 (2)	0.0733 (10)
H37A	0.8272	0.1414	0.5208	0.110*
H37B	0.7315	0.0932	0.5040	0.110*
H37C	0.8090	0.0518	0.5820	0.110*
C38	0.5891 (3)	0.0470 (4)	0.5538 (3)	0.0970 (13)
H38A	0.5277	0.0277	0.5409	0.146*
H38B	0.6250	−0.0142	0.5837	0.146*
H38C	0.6022	0.0607	0.5027	0.146*
C39	0.5660 (2)	0.1415 (4)	0.6782 (3)	0.0887 (12)
H39A	0.5739	0.2112	0.7102	0.106*
H39B	0.5029	0.1301	0.6521	0.106*
C40	0.6021 (3)	0.0460 (4)	0.7373 (3)	0.0980 (13)
H40A	0.5883	−0.0245	0.7064	0.118*
H40B	0.5726	0.0451	0.7797	0.118*
C41	0.7014 (2)	0.0517 (3)	0.7807 (2)	0.0723 (9)
H41	0.7186	−0.0266	0.7971	0.087*
C42	0.7486 (2)	0.0802 (3)	0.7161 (2)	0.0638 (8)

H42A	0.8095	0.0998	0.7463	0.077*
H42B	0.7497	0.0126	0.6837	0.077*
C43	0.7321 (3)	0.1185 (3)	0.8639 (2)	0.0728 (9)
C44	0.6778 (4)	0.0904 (4)	0.9203 (3)	0.1142 (16)
H44A	0.7029	0.1270	0.9736	0.171*
H44B	0.6777	0.0101	0.9284	0.171*
H44C	0.6181	0.1162	0.8948	0.171*
C45	0.8294 (3)	0.0932 (5)	0.9099 (3)	0.1106 (16)
H45A	0.8644	0.1141	0.8750	0.166*
H45B	0.8366	0.0139	0.9224	0.166*
H45C	0.8486	0.1357	0.9612	0.166*
C46	0.6265 (5)	0.5741 (5)	0.6761 (2)	0.130 (2)
H46A	0.6138	0.6261	0.6292	0.156*
H46B	0.6359	0.4999	0.6558	0.156*
C47	0.5472 (4)	0.5689 (5)	0.7069 (3)	0.129 (2)
H47A	0.5324	0.6446	0.7201	0.155*
H47B	0.4968	0.5391	0.6627	0.155*
C48	0.5651 (3)	0.4957 (4)	0.7832 (3)	0.0962 (13)
H48A	0.5706	0.4180	0.7671	0.115*
H48B	0.5145	0.4997	0.8034	0.115*
C49	0.6481 (2)	0.5269 (3)	0.85516 (19)	0.0652 (8)
C50	0.7261 (2)	0.5344 (3)	0.82020 (17)	0.0591 (8)
H50	0.7304	0.4582	0.7989	0.071*
C51	0.7113 (4)	0.6115 (3)	0.7429 (3)	0.0961 (14)
C52	0.6325 (3)	0.6311 (4)	0.9024 (2)	0.0878 (12)
H52A	0.5882	0.6144	0.9283	0.132*
H52B	0.6128	0.6927	0.8638	0.132*
H52C	0.6867	0.6516	0.9448	0.132*
C53	0.7060 (6)	0.7397 (4)	0.7617 (4)	0.163 (3)
H53A	0.6483	0.7570	0.7649	0.245*
H53B	0.7165	0.7833	0.7176	0.245*
H53C	0.7500	0.7578	0.8141	0.245*
C54	0.7915 (5)	0.5928 (4)	0.7114 (4)	0.132 (2)
H54A	0.7904	0.5156	0.6918	0.158*
H54B	0.7860	0.6425	0.6642	0.158*
C55	0.8803 (6)	0.6148 (5)	0.7786 (6)	0.170 (4)
H55A	0.9275	0.6012	0.7548	0.205*
H55B	0.8832	0.6936	0.7952	0.205*
C56	0.8955 (3)	0.5416 (5)	0.8557 (4)	0.1105 (17)
H56	0.9443	0.5779	0.8991	0.133*
C57	0.8148 (2)	0.5528 (4)	0.8868 (2)	0.0848 (11)
H57A	0.8209	0.4985	0.9316	0.102*
H57B	0.8153	0.6277	0.9104	0.102*
C58	0.9275 (3)	0.4200 (4)	0.8492 (3)	0.1035 (17)
C59	0.9977 (3)	0.4144 (6)	0.8058 (4)	0.157 (3)
H59A	1.0236	0.3403	0.8130	0.236*
H59B	1.0427	0.4696	0.8300	0.236*
H59C	0.9710	0.4297	0.7471	0.236*
C60	0.9640 (3)	0.3690 (6)	0.9367 (3)	0.140 (2)

H60A	0.9175	0.3635	0.9615	0.210*
H60B	1.0105	0.4163	0.9709	0.210*
H60C	0.9871	0.2949	0.9328	0.210*
O1	0.63823 (14)	0.48147 (18)	0.07659 (12)	0.0608 (5)
H1	0.6558	0.4674	0.0367	0.091*
O2	0.89726 (12)	0.52150 (18)	0.26048 (12)	0.0569 (5)
H2	0.8502	0.5489	0.2315	0.085*
O3	0.98669 (12)	0.70426 (19)	0.36327 (12)	0.0591 (5)
H3	0.9632	0.6546	0.3295	0.089*
O4	0.72952 (14)	0.64359 (17)	0.19505 (14)	0.0673 (6)
H4	0.7039	0.6049	0.1540	0.101*
O5	0.84756 (14)	0.2485 (3)	0.65677 (15)	0.0839 (8)
H5A	0.8875	0.2360	0.6370	0.126*
O6	0.72197 (16)	0.23920 (18)	0.84929 (16)	0.0717 (6)
H6	0.7670	0.2649	0.8424	0.108*
O7	0.66567 (19)	0.4394 (2)	0.91711 (16)	0.0796 (7)
H7	0.6803	0.3815	0.8980	0.119*
O8	0.85525 (14)	0.3481 (2)	0.80475 (16)	0.0792 (7)
H8	0.8661	0.3190	0.7648	0.119*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.100 (3)	0.082 (2)	0.066 (2)	−0.026 (2)	0.036 (2)	0.0105 (19)
C2	0.085 (3)	0.098 (3)	0.089 (2)	−0.031 (2)	0.048 (2)	−0.010 (2)
C3	0.0474 (16)	0.087 (2)	0.080 (2)	−0.0109 (16)	0.0222 (16)	−0.011 (2)
C4	0.0459 (15)	0.0559 (17)	0.0508 (15)	−0.0113 (13)	0.0109 (13)	−0.0053 (13)
C5	0.0455 (14)	0.0396 (13)	0.0458 (14)	−0.0085 (11)	0.0105 (12)	−0.0073 (11)
C6	0.074 (2)	0.0465 (16)	0.0602 (18)	−0.0123 (14)	0.0130 (16)	0.0069 (14)
C7	0.0642 (19)	0.086 (2)	0.0674 (19)	−0.0232 (18)	0.0012 (16)	−0.0189 (19)
C8	0.123 (3)	0.0460 (19)	0.113 (3)	−0.020 (2)	0.020 (3)	0.006 (2)
C9	0.085 (2)	0.062 (2)	0.065 (2)	0.0019 (17)	0.0003 (18)	0.0194 (17)
C10	0.068 (2)	0.065 (2)	0.108 (3)	0.0126 (17)	−0.003 (2)	0.002 (2)
C11	0.0465 (15)	0.0650 (19)	0.0682 (19)	0.0054 (13)	0.0144 (14)	−0.0217 (16)
C12	0.0502 (15)	0.0601 (18)	0.0539 (16)	−0.0048 (13)	0.0119 (13)	−0.0182 (14)
C13	0.0458 (16)	0.070 (2)	0.0690 (19)	−0.0069 (14)	0.0209 (14)	−0.0200 (16)
C14	0.138 (4)	0.096 (3)	0.096 (3)	−0.030 (3)	0.068 (3)	−0.017 (3)
C15	0.0429 (18)	0.112 (3)	0.151 (4)	−0.006 (2)	0.021 (2)	−0.049 (3)
C16	0.081 (2)	0.067 (2)	0.073 (2)	−0.0101 (17)	0.0434 (18)	−0.0032 (17)
C17	0.099 (3)	0.0596 (19)	0.0579 (17)	0.0069 (18)	0.0263 (18)	0.0043 (15)
C18	0.0574 (17)	0.0544 (17)	0.0552 (16)	0.0063 (13)	0.0104 (14)	0.0034 (14)
C19	0.0460 (14)	0.0456 (14)	0.0477 (14)	−0.0060 (12)	0.0098 (12)	−0.0042 (12)
C20	0.0473 (14)	0.0309 (12)	0.0545 (15)	−0.0034 (10)	0.0105 (12)	−0.0076 (11)
C21	0.0536 (16)	0.0560 (17)	0.0737 (19)	−0.0022 (13)	0.0275 (15)	−0.0146 (16)
C22	0.0639 (19)	0.066 (2)	0.071 (2)	−0.0212 (16)	0.0058 (16)	−0.0146 (17)
C23	0.102 (3)	0.082 (3)	0.097 (3)	0.015 (2)	0.048 (2)	−0.023 (2)
C24	0.0501 (18)	0.092 (3)	0.104 (3)	0.0003 (17)	0.0271 (19)	−0.005 (2)
C25	0.057 (2)	0.100 (3)	0.115 (3)	0.021 (2)	0.011 (2)	−0.010 (3)

C26	0.068 (2)	0.0409 (16)	0.084 (2)	0.0126 (14)	−0.0068 (18)	−0.0010 (15)
C27	0.0660 (18)	0.0385 (15)	0.0683 (19)	−0.0035 (13)	0.0020 (15)	0.0011 (14)
C28	0.074 (2)	0.0449 (16)	0.078 (2)	0.0087 (15)	−0.0107 (18)	0.0028 (16)
C29	0.106 (3)	0.106 (4)	0.134 (4)	0.053 (3)	−0.059 (3)	−0.037 (3)
C30	0.199 (6)	0.079 (3)	0.087 (3)	−0.030 (3)	0.032 (3)	0.003 (2)
C31	0.071 (2)	0.126 (4)	0.086 (3)	0.039 (2)	0.016 (2)	0.009 (3)
C32	0.116 (4)	0.122 (4)	0.090 (3)	0.050 (3)	0.029 (3)	0.024 (3)
C33	0.128 (4)	0.071 (2)	0.082 (2)	0.000 (2)	0.053 (3)	−0.001 (2)
C34	0.0525 (16)	0.0662 (19)	0.0636 (17)	−0.0063 (14)	0.0234 (14)	−0.0188 (16)
C35	0.0414 (14)	0.0494 (15)	0.0576 (15)	0.0016 (11)	0.0164 (12)	−0.0145 (13)
C36	0.0435 (16)	0.089 (3)	0.077 (2)	0.0035 (16)	0.0166 (15)	−0.0115 (19)
C37	0.0618 (19)	0.090 (3)	0.071 (2)	0.0029 (18)	0.0251 (16)	−0.0288 (19)
C38	0.069 (2)	0.115 (3)	0.101 (3)	−0.032 (2)	0.017 (2)	−0.037 (3)
C39	0.0396 (16)	0.124 (3)	0.107 (3)	−0.011 (2)	0.0286 (18)	−0.017 (3)
C40	0.098 (3)	0.100 (3)	0.109 (3)	−0.033 (3)	0.051 (3)	−0.007 (3)
C41	0.090 (2)	0.0442 (16)	0.087 (2)	0.0043 (16)	0.036 (2)	0.0007 (17)
C42	0.0597 (18)	0.0579 (19)	0.077 (2)	0.0112 (14)	0.0257 (16)	−0.0063 (16)
C43	0.094 (3)	0.0521 (18)	0.082 (2)	0.0096 (17)	0.041 (2)	0.0029 (17)
C44	0.172 (5)	0.089 (3)	0.109 (3)	−0.001 (3)	0.083 (4)	0.003 (3)
C45	0.125 (4)	0.100 (3)	0.088 (3)	0.038 (3)	0.007 (3)	0.004 (3)
C46	0.227 (6)	0.106 (4)	0.052 (2)	0.084 (4)	0.038 (3)	0.018 (2)
C47	0.149 (5)	0.134 (5)	0.081 (3)	0.076 (4)	0.002 (3)	−0.011 (3)
C48	0.080 (3)	0.097 (3)	0.103 (3)	0.029 (2)	0.017 (2)	−0.019 (3)
C49	0.081 (2)	0.0581 (18)	0.0635 (18)	0.0217 (16)	0.0325 (17)	0.0076 (15)
C50	0.091 (2)	0.0457 (15)	0.0494 (15)	0.0049 (15)	0.0338 (16)	−0.0045 (13)
C51	0.187 (5)	0.0460 (19)	0.075 (2)	0.019 (2)	0.070 (3)	0.0106 (17)
C52	0.124 (3)	0.078 (2)	0.073 (2)	0.039 (2)	0.047 (2)	0.0021 (19)
C53	0.333 (10)	0.045 (2)	0.164 (5)	0.025 (4)	0.154 (6)	0.020 (3)
C54	0.254 (8)	0.071 (3)	0.127 (4)	0.002 (4)	0.141 (5)	0.018 (3)
C55	0.233 (8)	0.093 (4)	0.267 (9)	−0.069 (5)	0.195 (8)	−0.056 (5)
C56	0.099 (3)	0.102 (3)	0.147 (4)	−0.048 (3)	0.063 (3)	−0.068 (3)
C57	0.092 (3)	0.084 (3)	0.088 (2)	−0.013 (2)	0.041 (2)	−0.041 (2)
C58	0.068 (2)	0.119 (4)	0.131 (4)	−0.033 (2)	0.042 (3)	−0.076 (3)
C59	0.090 (3)	0.170 (6)	0.248 (7)	−0.058 (4)	0.104 (4)	−0.110 (6)
C60	0.094 (3)	0.173 (6)	0.129 (4)	0.001 (3)	0.000 (3)	−0.071 (4)
O1	0.0598 (12)	0.0645 (13)	0.0505 (11)	−0.0003 (9)	0.0068 (10)	0.0008 (10)
O2	0.0439 (10)	0.0599 (12)	0.0641 (11)	−0.0045 (9)	0.0132 (9)	−0.0191 (10)
O3	0.0461 (11)	0.0701 (14)	0.0595 (12)	−0.0143 (9)	0.0146 (9)	−0.0058 (10)
O4	0.0627 (12)	0.0423 (11)	0.0757 (14)	0.0066 (9)	−0.0081 (10)	−0.0071 (10)
O5	0.0597 (13)	0.120 (2)	0.0855 (15)	−0.0316 (14)	0.0418 (12)	−0.0509 (16)
O6	0.0820 (16)	0.0516 (13)	0.0906 (16)	0.0060 (10)	0.0403 (13)	−0.0088 (11)
O7	0.1116 (19)	0.0693 (15)	0.0801 (16)	0.0293 (13)	0.0617 (15)	0.0197 (12)
O8	0.0658 (13)	0.0847 (17)	0.0968 (18)	−0.0201 (12)	0.0395 (13)	−0.0470 (14)

Geometric parameters (Å, °)

C1—C2	1.508 (5)	C32—C33	1.517 (6)
C1—C6	1.531 (5)	C32—H32A	0.9700
C1—H1A	0.9700	C32—H32B	0.9700

C1—H1B	0.9700	C33—C34	1.518 (5)
C2—C3	1.509 (6)	C33—H33A	0.9700
C2—H2A	0.9700	C33—H33B	0.9700
C2—H2B	0.9700	C34—O5	1.438 (4)
C3—C4	1.519 (4)	C34—C37	1.523 (4)
C3—H3A	0.9700	C34—C35	1.546 (4)
C3—H3B	0.9700	C35—C42	1.525 (4)
C4—O1	1.447 (4)	C35—C36	1.541 (4)
C4—C7	1.524 (4)	C35—H35	0.9800
C4—C5	1.533 (4)	C36—C39	1.537 (5)
C5—C12	1.526 (4)	C36—C38	1.551 (6)
C5—C6	1.547 (4)	C37—H37A	0.9600
C5—H5	0.9800	C37—H37B	0.9600
C6—C9	1.531 (5)	C37—H37C	0.9600
C6—C8	1.548 (5)	C38—H38A	0.9600
C7—H7A	0.9600	C38—H38B	0.9600
C7—H7B	0.9600	C38—H38C	0.9600
C7—H7C	0.9600	C39—C40	1.494 (7)
C8—H8A	0.9600	C39—H39A	0.9700
C8—H8B	0.9600	C39—H39B	0.9700
C8—H8C	0.9600	C40—C41	1.518 (5)
C9—C10	1.513 (5)	C40—H40A	0.9700
C9—H9A	0.9700	C40—H40B	0.9700
C9—H9B	0.9700	C41—C42	1.542 (5)
C10—C11	1.526 (5)	C41—C43	1.544 (5)
C10—H10A	0.9700	C41—H41	0.9800
C10—H10B	0.9700	C42—H42A	0.9700
C11—C12	1.535 (4)	C42—H42B	0.9700
C11—C13	1.550 (5)	C43—O6	1.449 (4)
C11—H11	0.9800	C43—C44	1.510 (6)
C12—H12A	0.9700	C43—C45	1.526 (6)
C12—H12B	0.9700	C44—H44A	0.9600
C13—O2	1.439 (4)	C44—H44B	0.9600
C13—C14	1.512 (5)	C44—H44C	0.9600
C13—C15	1.527 (5)	C45—H45A	0.9600
C14—H14A	0.9600	C45—H45B	0.9600
C14—H14B	0.9600	C45—H45C	0.9600
C14—H14C	0.9600	C46—C47	1.511 (8)
C15—H15A	0.9600	C46—C51	1.522 (8)
C15—H15B	0.9600	C46—H46A	0.9700
C15—H15C	0.9600	C46—H46B	0.9700
C16—C17	1.514 (5)	C47—C48	1.498 (7)
C16—C21	1.531 (5)	C47—H47A	0.9700
C16—H16A	0.9700	C47—H47B	0.9700
C16—H16B	0.9700	C48—C49	1.526 (5)
C17—C18	1.512 (5)	C48—H48A	0.9700
C17—H17A	0.9700	C48—H48B	0.9700
C17—H17B	0.9700	C49—O7	1.431 (4)
C18—C19	1.531 (4)	C49—C52	1.529 (5)

C18—H18A	0.9700	C49—C50	1.536 (4)
C18—H18B	0.9700	C50—C57	1.515 (5)
C19—O3	1.449 (3)	C50—C51	1.542 (5)
C19—C22	1.524 (4)	C50—H50	0.9800
C19—C20	1.539 (4)	C51—C54	1.546 (7)
C20—C27	1.528 (4)	C51—C53	1.557 (6)
C20—C21	1.550 (4)	C52—H52A	0.9600
C20—H20	0.9800	C52—H52B	0.9600
C21—C24	1.529 (5)	C52—H52C	0.9600
C21—C23	1.541 (5)	C53—H53A	0.9600
C22—H22A	0.9600	C53—H53B	0.9600
C22—H22B	0.9600	C53—H53C	0.9600
C22—H22C	0.9600	C54—C55	1.526 (9)
C23—H23A	0.9600	C54—H54A	0.9700
C23—H23B	0.9600	C54—H54B	0.9700
C23—H23C	0.9600	C55—C56	1.513 (10)
C24—C25	1.505 (6)	C55—H55A	0.9700
C24—H24A	0.9700	C55—H55B	0.9700
C24—H24B	0.9700	C56—C57	1.539 (6)
C25—C26	1.529 (6)	C56—C58	1.541 (7)
C25—H25A	0.9700	C56—H56	0.9800
C25—H25B	0.9700	C57—H57A	0.9700
C26—C28	1.542 (5)	C57—H57B	0.9700
C26—C27	1.543 (4)	C58—O8	1.435 (4)
C26—H26	0.9800	C58—C59	1.519 (6)
C27—H27A	0.9700	C58—C60	1.523 (8)
C27—H27B	0.9700	C59—H59A	0.9600
C28—O4	1.431 (4)	C59—H59B	0.9600
C28—C29	1.528 (5)	C59—H59C	0.9600
C28—C30	1.533 (7)	C60—H60A	0.9600
C29—H29A	0.9600	C60—H60B	0.9600
C29—H29B	0.9600	C60—H60C	0.9600
C29—H29C	0.9600	O1—H1	0.8200
C30—H30A	0.9600	O2—H2	0.8200
C30—H30B	0.9600	O3—H3	0.8200
C30—H30C	0.9600	O4—H4	0.8200
C31—C36	1.517 (6)	O5—H5A	0.8200
C31—C32	1.536 (6)	O6—H6	0.8200
C31—H31A	0.9700	O7—H7	0.8200
C31—H31B	0.9700	O8—H8	0.8200
C2—C1—C6	113.9 (3)	C32—C31—H31B	109.0
C2—C1—H1A	108.8	H31A—C31—H31B	107.8
C6—C1—H1A	108.8	C33—C32—C31	111.1 (3)
C2—C1—H1B	108.8	C33—C32—H32A	109.4
C6—C1—H1B	108.8	C31—C32—H32A	109.4
H1A—C1—H1B	107.7	C33—C32—H32B	109.4
C1—C2—C3	111.1 (3)	C31—C32—H32B	109.4
C1—C2—H2A	109.4	H32A—C32—H32B	108.0
C3—C2—H2A	109.4	C32—C33—C34	114.8 (4)

C1—C2—H2B	109.4	C32—C33—H33A	108.6
C3—C2—H2B	109.4	C34—C33—H33A	108.6
H2A—C2—H2B	108.0	C32—C33—H33B	108.6
C2—C3—C4	113.1 (3)	C34—C33—H33B	108.6
C2—C3—H3A	109.0	H33A—C33—H33B	107.5
C4—C3—H3A	109.0	O5—C34—C33	108.7 (3)
C2—C3—H3B	109.0	O5—C34—C37	107.8 (2)
C4—C3—H3B	109.0	C33—C34—C37	111.0 (3)
H3A—C3—H3B	107.8	O5—C34—C35	105.2 (2)
O1—C4—C3	104.7 (2)	C33—C34—C35	108.5 (3)
O1—C4—C7	107.5 (2)	C37—C34—C35	115.4 (3)
C3—C4—C7	111.6 (2)	C42—C35—C36	111.4 (3)
O1—C4—C5	107.7 (2)	C42—C35—C34	113.6 (2)
C3—C4—C5	109.6 (2)	C36—C35—C34	116.1 (2)
C7—C4—C5	115.2 (3)	C42—C35—H35	104.8
C12—C5—C4	114.2 (2)	C36—C35—H35	104.8
C12—C5—C6	112.4 (2)	C34—C35—H35	104.8
C4—C5—C6	116.2 (2)	C31—C36—C39	110.0 (3)
C12—C5—H5	104.1	C31—C36—C35	109.3 (3)
C4—C5—H5	104.1	C39—C36—C35	105.7 (3)
C6—C5—H5	104.1	C31—C36—C38	109.3 (3)
C1—C6—C9	109.9 (3)	C39—C36—C38	108.0 (3)
C1—C6—C5	107.6 (3)	C35—C36—C38	114.5 (3)
C9—C6—C5	106.0 (2)	C34—C37—H37A	109.5
C1—C6—C8	109.9 (3)	C34—C37—H37B	109.5
C9—C6—C8	108.6 (3)	H37A—C37—H37B	109.5
C5—C6—C8	114.8 (3)	C34—C37—H37C	109.5
C4—C7—H7A	109.5	H37A—C37—H37C	109.5
C4—C7—H7B	109.5	H37B—C37—H37C	109.5
H7A—C7—H7B	109.5	C36—C38—H38A	109.5
C4—C7—H7C	109.5	C36—C38—H38B	109.5
H7A—C7—H7C	109.5	H38A—C38—H38B	109.5
H7B—C7—H7C	109.5	C36—C38—H38C	109.5
C6—C8—H8A	109.5	H38A—C38—H38C	109.5
C6—C8—H8B	109.5	H38B—C38—H38C	109.5
H8A—C8—H8B	109.5	C40—C39—C36	114.3 (3)
C6—C8—H8C	109.5	C40—C39—H39A	108.7
H8A—C8—H8C	109.5	C36—C39—H39A	108.7
H8B—C8—H8C	109.5	C40—C39—H39B	108.7
C10—C9—C6	113.8 (3)	C36—C39—H39B	108.7
C10—C9—H9A	108.8	H39A—C39—H39B	107.6
C6—C9—H9A	108.8	C39—C40—C41	114.1 (3)
C10—C9—H9B	108.8	C39—C40—H40A	108.7
C6—C9—H9B	108.8	C41—C40—H40A	108.7
H9A—C9—H9B	107.7	C39—C40—H40B	108.7
C9—C10—C11	114.5 (3)	C41—C40—H40B	108.7
C9—C10—H10A	108.6	H40A—C40—H40B	107.6
C11—C10—H10A	108.6	C40—C41—C42	109.7 (3)
C9—C10—H10B	108.6	C40—C41—C43	116.1 (3)

C11—C10—H10B	108.6	C42—C41—C43	116.1 (3)
H10A—C10—H10B	107.6	C40—C41—H41	104.4
C10—C11—C12	108.9 (3)	C42—C41—H41	104.4
C10—C11—C13	115.4 (3)	C43—C41—H41	104.4
C12—C11—C13	115.2 (3)	C35—C42—C41	116.2 (2)
C10—C11—H11	105.4	C35—C42—H42A	108.2
C12—C11—H11	105.4	C41—C42—H42A	108.2
C13—C11—H11	105.4	C35—C42—H42B	108.2
C5—C12—C11	113.9 (2)	C41—C42—H42B	108.2
C5—C12—H12A	108.8	H42A—C42—H42B	107.4
C11—C12—H12A	108.8	O6—C43—C44	105.6 (3)
C5—C12—H12B	108.8	O6—C43—C45	108.7 (3)
C11—C12—H12B	108.8	C44—C43—C45	109.4 (4)
H12A—C12—H12B	107.7	O6—C43—C41	111.4 (3)
O2—C13—C14	107.6 (3)	C44—C43—C41	112.1 (3)
O2—C13—C15	103.7 (3)	C45—C43—C41	109.7 (3)
C14—C13—C15	109.6 (3)	C43—C44—H44A	109.5
O2—C13—C11	113.1 (2)	C43—C44—H44B	109.5
C14—C13—C11	111.8 (3)	H44A—C44—H44B	109.5
C15—C13—C11	110.6 (3)	C43—C44—H44C	109.5
C13—C14—H14A	109.5	H44A—C44—H44C	109.5
C13—C14—H14B	109.5	H44B—C44—H44C	109.5
H14A—C14—H14B	109.5	C43—C45—H45A	109.5
C13—C14—H14C	109.5	C43—C45—H45B	109.5
H14A—C14—H14C	109.5	H45A—C45—H45B	109.5
H14B—C14—H14C	109.5	C43—C45—H45C	109.5
C13—C15—H15A	109.5	H45A—C45—H45C	109.5
C13—C15—H15B	109.5	H45B—C45—H45C	109.5
H15A—C15—H15B	109.5	C47—C46—C51	113.7 (3)
C13—C15—H15C	109.5	C47—C46—H46A	108.8
H15A—C15—H15C	109.5	C51—C46—H46A	108.8
H15B—C15—H15C	109.5	C47—C46—H46B	108.8
C17—C16—C21	112.7 (3)	C51—C46—H46B	108.8
C17—C16—H16A	109.1	H46A—C46—H46B	107.7
C21—C16—H16A	109.1	C48—C47—C46	111.3 (4)
C17—C16—H16B	109.1	C48—C47—H47A	109.4
C21—C16—H16B	109.1	C46—C47—H47A	109.4
H16A—C16—H16B	107.8	C48—C47—H47B	109.4
C18—C17—C16	110.1 (2)	C46—C47—H47B	109.4
C18—C17—H17A	109.6	H47A—C47—H47B	108.0
C16—C17—H17A	109.6	C47—C48—C49	114.9 (4)
C18—C17—H17B	109.6	C47—C48—H48A	108.5
C16—C17—H17B	109.6	C49—C48—H48A	108.5
H17A—C17—H17B	108.2	C47—C48—H48B	108.5
C17—C18—C19	114.3 (2)	C49—C48—H48B	108.5
C17—C18—H18A	108.7	H48A—C48—H48B	107.5
C19—C18—H18A	108.7	O7—C49—C48	108.8 (3)
C17—C18—H18B	108.7	O7—C49—C52	103.4 (2)
C19—C18—H18B	108.7	C48—C49—C52	111.3 (3)

H18A—C18—H18B	107.6	O7—C49—C50	108.9 (2)
O3—C19—C22	103.7 (2)	C48—C49—C50	108.2 (3)
O3—C19—C18	107.9 (2)	C52—C49—C50	115.9 (3)
C22—C19—C18	111.5 (2)	C57—C50—C49	113.8 (2)
O3—C19—C20	108.6 (2)	C57—C50—C51	113.3 (3)
C22—C19—C20	114.9 (2)	C49—C50—C51	115.5 (3)
C18—C19—C20	109.8 (2)	C57—C50—H50	104.2
C27—C20—C19	114.1 (2)	C49—C50—H50	104.2
C27—C20—C21	112.2 (2)	C51—C50—H50	104.2
C19—C20—C21	115.8 (2)	C46—C51—C50	108.2 (4)
C27—C20—H20	104.4	C46—C51—C54	110.0 (4)
C19—C20—H20	104.4	C50—C51—C54	106.3 (4)
C21—C20—H20	104.4	C46—C51—C53	109.9 (5)
C24—C21—C16	109.0 (3)	C50—C51—C53	114.1 (3)
C24—C21—C23	109.2 (3)	C54—C51—C53	108.2 (4)
C16—C21—C23	109.1 (3)	C49—C52—H52A	109.5
C24—C21—C20	105.7 (2)	C49—C52—H52B	109.5
C16—C21—C20	108.6 (2)	H52A—C52—H52B	109.5
C23—C21—C20	115.1 (3)	C49—C52—H52C	109.5
C19—C22—H22A	109.5	H52A—C52—H52C	109.5
C19—C22—H22B	109.5	H52B—C52—H52C	109.5
H22A—C22—H22B	109.5	C51—C53—H53A	109.5
C19—C22—H22C	109.5	C51—C53—H53B	109.5
H22A—C22—H22C	109.5	H53A—C53—H53B	109.5
H22B—C22—H22C	109.5	C51—C53—H53C	109.5
C21—C23—H23A	109.5	H53A—C53—H53C	109.5
C21—C23—H23B	109.5	H53B—C53—H53C	109.5
H23A—C23—H23B	109.5	C55—C54—C51	113.3 (4)
C21—C23—H23C	109.5	C55—C54—H54A	108.9
H23A—C23—H23C	109.5	C51—C54—H54A	108.9
H23B—C23—H23C	109.5	C55—C54—H54B	108.9
C25—C24—C21	113.3 (3)	C51—C54—H54B	108.9
C25—C24—H24A	108.9	H54A—C54—H54B	107.7
C21—C24—H24A	108.9	C56—C55—C54	113.3 (4)
C25—C24—H24B	108.9	C56—C55—H55A	108.9
C21—C24—H24B	108.9	C54—C55—H55A	108.9
H24A—C24—H24B	107.7	C56—C55—H55B	108.9
C24—C25—C26	115.2 (3)	C54—C55—H55B	108.9
C24—C25—H25A	108.5	H55A—C55—H55B	107.7
C26—C25—H25A	108.5	C55—C56—C57	108.5 (5)
C24—C25—H25B	108.5	C55—C56—C58	116.1 (4)
C26—C25—H25B	108.5	C57—C56—C58	115.8 (4)
H25A—C25—H25B	107.5	C55—C56—H56	105.1
C25—C26—C28	116.9 (3)	C57—C56—H56	105.1
C25—C26—C27	109.4 (3)	C58—C56—H56	105.1
C28—C26—C27	114.3 (3)	C50—C57—C56	114.9 (3)
C25—C26—H26	105.0	C50—C57—H57A	108.5
C28—C26—H26	105.0	C56—C57—H57A	108.5
C27—C26—H26	105.0	C50—C57—H57B	108.5

C20—C27—C26	114.1 (2)	C56—C57—H57B	108.5
C20—C27—H27A	108.7	H57A—C57—H57B	107.5
C26—C27—H27A	108.7	O8—C58—C59	108.3 (3)
C20—C27—H27B	108.7	O8—C58—C60	105.4 (4)
C26—C27—H27B	108.7	C59—C58—C60	109.4 (5)
H27A—C27—H27B	107.6	O8—C58—C56	111.2 (4)
O4—C28—C29	108.0 (3)	C59—C58—C56	112.6 (5)
O4—C28—C30	106.3 (4)	C60—C58—C56	109.6 (4)
C29—C28—C30	109.5 (4)	C58—C59—H59A	109.5
O4—C28—C26	110.4 (3)	C58—C59—H59B	109.5
C29—C28—C26	111.2 (3)	H59A—C59—H59B	109.5
C30—C28—C26	111.2 (3)	C58—C59—H59C	109.5
C28—C29—H29A	109.5	H59A—C59—H59C	109.5
C28—C29—H29B	109.5	H59B—C59—H59C	109.5
H29A—C29—H29B	109.5	C58—C60—H60A	109.5
C28—C29—H29C	109.5	C58—C60—H60B	109.5
H29A—C29—H29C	109.5	H60A—C60—H60B	109.5
H29B—C29—H29C	109.5	C58—C60—H60C	109.5
C28—C30—H30A	109.5	H60A—C60—H60C	109.5
C28—C30—H30B	109.5	H60B—C60—H60C	109.5
H30A—C30—H30B	109.5	C4—O1—H1	109.5
C28—C30—H30C	109.5	C13—O2—H2	109.5
H30A—C30—H30C	109.5	C19—O3—H3	109.5
H30B—C30—H30C	109.5	C28—O4—H4	109.5
C36—C31—C32	112.9 (3)	C34—O5—H5A	109.5
C36—C31—H31A	109.0	C43—O6—H6	109.5
C32—C31—H31A	109.0	C49—O7—H7	109.5
C36—C31—H31B	109.0	C58—O8—H8	109.5
C6—C1—C2—C3	−57.0 (4)	C36—C31—C32—C33	−54.6 (6)
C1—C2—C3—C4	55.8 (4)	C31—C32—C33—C34	54.4 (5)
C2—C3—C4—O1	−167.4 (3)	C32—C33—C34—O5	−165.2 (3)
C2—C3—C4—C7	76.7 (3)	C32—C33—C34—C37	76.4 (4)
C2—C3—C4—C5	−52.1 (3)	C32—C33—C34—C35	−51.4 (4)
O1—C4—C5—C12	−61.9 (3)	O5—C34—C35—C42	−61.4 (3)
C3—C4—C5—C12	−175.2 (3)	C33—C34—C35—C42	−177.6 (3)
C7—C4—C5—C12	58.1 (3)	C37—C34—C35—C42	57.2 (3)
O1—C4—C5—C6	164.8 (2)	O5—C34—C35—C36	167.5 (3)
C3—C4—C5—C6	51.5 (3)	C33—C34—C35—C36	51.3 (4)
C7—C4—C5—C6	−75.3 (3)	C37—C34—C35—C36	−73.9 (3)
C2—C1—C6—C9	167.9 (3)	C32—C31—C36—C39	168.4 (4)
C2—C1—C6—C5	52.9 (4)	C32—C31—C36—C35	52.9 (5)
C2—C1—C6—C8	−72.7 (4)	C32—C31—C36—C38	−73.1 (5)
C12—C5—C6—C1	174.7 (2)	C42—C35—C36—C31	175.0 (3)
C4—C5—C6—C1	−51.2 (3)	C34—C35—C36—C31	−52.9 (4)
C12—C5—C6—C9	57.1 (3)	C42—C35—C36—C39	56.7 (4)
C4—C5—C6—C9	−168.7 (3)	C34—C35—C36—C39	−171.1 (3)
C12—C5—C6—C8	−62.7 (4)	C42—C35—C36—C38	−62.0 (4)
C4—C5—C6—C8	71.4 (4)	C34—C35—C36—C38	70.1 (4)
C1—C6—C9—C10	−172.6 (3)	C31—C36—C39—C40	−177.6 (4)

C5—C6—C9—C10	−56.6 (4)	C35—C36—C39—C40	−59.8 (4)
C8—C6—C9—C10	67.2 (4)	C38—C36—C39—C40	63.2 (4)
C6—C9—C10—C11	55.8 (4)	C36—C39—C40—C41	56.7 (5)
C9—C10—C11—C12	−49.1 (4)	C39—C40—C41—C42	−45.7 (4)
C9—C10—C11—C13	82.2 (4)	C39—C40—C41—C43	88.5 (4)
C4—C5—C12—C11	167.5 (2)	C36—C35—C42—C41	−53.8 (3)
C6—C5—C12—C11	−57.4 (3)	C34—C35—C42—C41	172.8 (3)
C10—C11—C12—C5	50.2 (3)	C40—C41—C42—C35	45.6 (4)
C13—C11—C12—C5	−81.3 (4)	C43—C41—C42—C35	−88.6 (4)
C10—C11—C13—O2	−61.9 (3)	C40—C41—C43—O6	−73.2 (4)
C12—C11—C13—O2	66.4 (4)	C42—C41—C43—O6	58.0 (4)
C10—C11—C13—C14	176.5 (3)	C40—C41—C43—C44	44.7 (4)
C12—C11—C13—C14	−55.3 (4)	C42—C41—C43—C44	176.0 (3)
C10—C11—C13—C15	54.0 (4)	C40—C41—C43—C45	166.4 (4)
C12—C11—C13—C15	−177.8 (3)	C42—C41—C43—C45	−62.3 (4)
C21—C16—C17—C18	−58.9 (4)	C51—C46—C47—C48	−54.7 (6)
C16—C17—C18—C19	56.1 (4)	C46—C47—C48—C49	53.8 (5)
C17—C18—C19—O3	−168.4 (2)	C47—C48—C49—O7	−169.8 (3)
C17—C18—C19—C22	78.3 (3)	C47—C48—C49—C52	76.8 (4)
C17—C18—C19—C20	−50.2 (3)	C47—C48—C49—C50	−51.6 (4)
O3—C19—C20—C27	−61.2 (3)	O7—C49—C50—C57	−55.8 (4)
C22—C19—C20—C27	54.4 (3)	C48—C49—C50—C57	−174.0 (3)
C18—C19—C20—C27	−179.0 (2)	C52—C49—C50—C57	60.2 (4)
O3—C19—C20—C21	166.2 (2)	O7—C49—C50—C51	170.7 (3)
C22—C19—C20—C21	−78.2 (3)	C48—C49—C50—C51	52.5 (4)
C18—C19—C20—C21	48.5 (3)	C52—C49—C50—C51	−73.3 (4)
C17—C16—C21—C24	170.2 (3)	C47—C46—C51—C50	53.6 (5)
C17—C16—C21—C23	−70.7 (3)	C47—C46—C51—C54	169.4 (4)
C17—C16—C21—C20	55.5 (3)	C47—C46—C51—C53	−71.6 (5)
C27—C20—C21—C24	58.6 (3)	C57—C50—C51—C46	172.3 (3)
C19—C20—C21—C24	−168.0 (2)	C49—C50—C51—C46	−53.9 (4)
C27—C20—C21—C16	175.5 (2)	C57—C50—C51—C54	54.1 (4)
C19—C20—C21—C16	−51.2 (3)	C49—C50—C51—C54	−172.1 (4)
C27—C20—C21—C23	−62.0 (3)	C57—C50—C51—C53	−65.1 (6)
C19—C20—C21—C23	71.4 (3)	C49—C50—C51—C53	68.7 (6)
C16—C21—C24—C25	−174.9 (3)	C46—C51—C54—C55	−173.0 (4)
C23—C21—C24—C25	66.0 (4)	C50—C51—C54—C55	−56.1 (5)
C20—C21—C24—C25	−58.4 (4)	C53—C51—C54—C55	66.9 (6)
C21—C24—C25—C26	55.8 (4)	C51—C54—C55—C56	58.4 (6)
C24—C25—C26—C28	85.0 (4)	C54—C55—C56—C57	−51.9 (5)
C24—C25—C26—C27	−47.0 (4)	C54—C55—C56—C58	80.5 (6)
C19—C20—C27—C26	169.5 (3)	C49—C50—C57—C56	170.6 (4)
C21—C20—C27—C26	−56.2 (3)	C51—C50—C57—C56	−54.8 (5)
C25—C26—C27—C20	47.3 (4)	C55—C56—C57—C50	50.9 (5)
C28—C26—C27—C20	−86.1 (4)	C58—C56—C57—C50	−81.7 (6)
C25—C26—C28—O4	−68.8 (4)	C55—C56—C58—O8	−79.6 (5)
C27—C26—C28—O4	60.9 (4)	C57—C56—C58—O8	49.3 (6)
C25—C26—C28—C29	51.1 (5)	C55—C56—C58—C59	42.2 (6)
C27—C26—C28—C29	−179.2 (4)	C57—C56—C58—C59	171.2 (4)

C25—C26—C28—C30	173.4 (3)	C55—C56—C58—C60	164.2 (5)
C27—C26—C28—C30	−56.9 (4)	C57—C56—C58—C60	−66.8 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O7^{i}	0.82	2.09	2.892 (3)	165
O5—H5A···O3^{ii}	0.82	2.04	2.815 (3)	158
O2—H2···O4	0.82	2.14	2.927 (3)	161
O3—H3···O2	0.82	2.04	2.851 (3)	171
O4—H4···O1	0.82	2.01	2.814 (3)	165
O6—H6···O8	0.82	1.98	2.782 (3)	166
O7—H7···O6	0.82	2.07	2.891 (3)	178
O8—H8···O5	0.82	1.93	2.719 (3)	160
C5—H5···O2	0.98	2.48	3.221 (3)	132
C5—H5···O4	0.98	2.59	3.422 (3)	143
C9—H9A···O2	0.97	2.59	3.201 (4)	121
C50—H50···O8	0.98	2.35	3.081 (4)	131
C20—H20···O4	0.98	2.44	3.163 (3)	130

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

Fig. 1

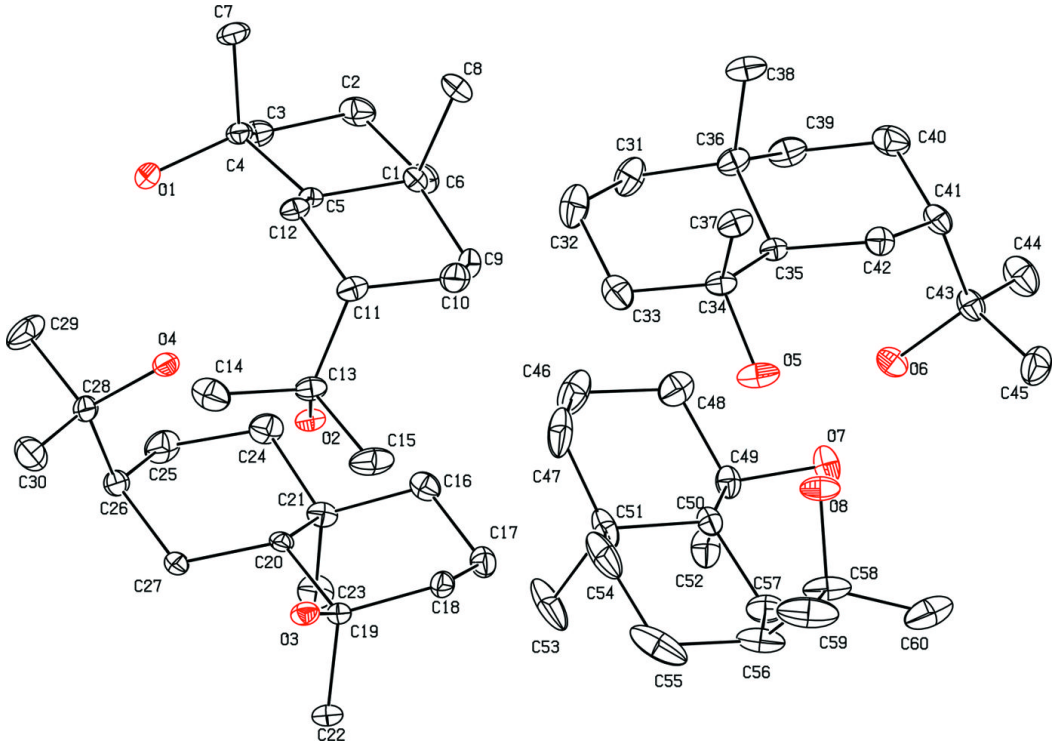
C7
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Fig. 2