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trans-(*R*,*R*)-2,2'-(Cyclopenta-1,2-diyl)diphenyl Bis[(*R*)-*O*-methylmandelate]

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Abstract

The title compound, $C_{35}H_{34}O_6$, crystallizes with two independent molecules per asymmetric unit. The molecules assume slightly different conformations. The crystallographically unique molecules stack in columns along the *b* axis. Close C—H···O contacts are observed between molecules related by a twofold screw axis. Such contacts are: C35—H35···O40 (related by $2 - x$, $1/2 + y$, $-1 - z$), C···O 3.440 (5) Å; H···O 2.553 (5) Å; C—H···O 153.7 (1)° for molecule 1 and: C33'-H33'···O40' (related by $1 - x$, $-1/2 + y$, $1 - z$); C···O 3.422 (5) Å, H···O 2.491 (5) Å, 163.3 (1)° for molecule 2. The absolute configuration was established by internal comparison to the (*R*)-(-)-*O*-methyl mandelic acid moiety.

Comment

The title compound, $C_{35}H_{34}O_6$, was prepared in enantiopure form (Whitesell and Apodaca, 1997) as a prototype of a new class of chiral C2-symmetric molecules (Whitesell, 1989). The intention is to use such molecules as chiral control elements. The immediate goal is to develop useful chiral ligands for enantioselective catalysis. Some of the most widely utilized chiral auxiliaries in enantioselective reactions are the 1,1'-binaphthalene-2,2'-diols and related molecules (Rosini *et al.*, 1992; Bao *et al.*, 1996). The synthesis and resolution of a molecule with a structure similar to the title compound, *trans*-4,5-bis(2-hydroxyphenyl)-2,2-dimethyl-1,3- dioxolane, has been reported (Yamamoto, Kobayashi and Kanemasa, 1996).

Experimental

The synthesis of the title compound is described in Whitesell and Apodaca, 1997.

Computing details

Data collection: *XSCANS* v2.10b, Siemens (1994); cell refinement: *XSCANS* v2.10b, Siemens (1994); data reduction: *XSCANS* v2.10b, Siemens (1994); program(s) used to solve structure: XS *SHELXTL/PC*, Sheldrick (1994); program(s) used to refine structure: XL *SHELXTL/PC*, Sheldrick (1994); molecular graphics: *XP SHELXTL/PC*, Sheldrick (1994).

(*R*,*R*)-*trans*-1,2-Bis(2-hydroxyphenyl)cyclopentane,bis(*R*)—*O*-methylmandelic acid ester

Crystal data

$C_{35}H_{34}O_6$	$V = 2908.8$ (5) Å^3
$M_r = 550.62$	$Z = 4$
Monoclinic, $P2_1$	Mo $K\alpha$
$a = 17.232$ (1) Å	$\mu = 0.09$ mm^{-1}

b = 7.294 (1) Å	T = 183 (2) K
c = 23.241 (2) Å	0.51 × 0.34 × 0.26 mm
β = 95.27 (1)º	

Data collection

Siemens P4 diffractometer	R_{int} = 0.033
Absorption correction: none	4 standard reflections
7811 measured reflections	every 96 reflections
7034 independent reflections	intensity decay: less than 1%
4357 reflections with $I > 2\sigma(I)$	

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052	H-atom parameters not refined
$wR(F^2)$ = 0.105	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
7032 reflections	Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881
741 parameters	Flack parameter: 1.99 (173)
1 restraint	

Acknowledgements

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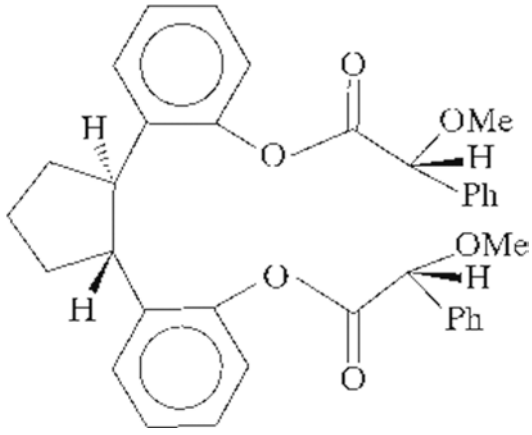
Scheme 1



supplementary materials

(*R*,*R*)-*trans*-1,2-Bis(2-hydroxyphenyl)cyclopentane,bis(*R*)—*O*-methylmandelic acid ester

Crystal data

$C_{35}H_{34}O_6$	F_{000} = 1168
M_r = 550.62	D_x = 1.26 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2y1	Cell parameters from 31 reflections
a = 17.232 (1) Å	θ = 11.6–12.5º
b = 7.294 (1) Å	μ = 0.09 mm^{-1}
c = 23.241 (2) Å	T = 183 (2) K
β = 95.27 (1)º	Block, colourless
V = 2908.8 (5) Å^3	0.51 × 0.34 × 0.26 mm
Z = 4	

Data collection

Siemens P4 diffractometer	R_{int} = 0.033
Radiation source: normal-focus sealed tube	θ_{max} = 27.5º
Monochromator: graphite	θ_{min} = 2.0º
T = 183(2) K	h = −1→16
ω scans	k = −1→9
Absorption correction: none	l = −30→30
7811 measured reflections	4 standard reflections
7034 independent reflections	every 96 reflections
4357 reflections with $I > 2\sigma(I)$	intensity decay: less than 1%

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters not refined
$R[F^2 > 2\sigma(F^2)]$ = 0.052	Calculated $w = 1/[\sigma^2(F_o^2) + (0.0378P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$?
$wR(F^2)$ = 0.105	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
7032 reflections	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
741 parameters	Extinction coefficient: 0.0153 (6)
1 restraint	Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881
Primary atom site location: structure-invariant direct methods	Flack parameter: 1.99 (173)
Secondary atom site location: difference Fourier map	

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 on F^2 for ALL reflections except for 2 with very negative F^2 or flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating _R_factor_obs *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	0.9001 (2)	0.7730 (6)	−0.2210 (2)	0.0298 (11)
H1	0.9315 (2)	0.7929 (6)	−0.1853 (2)	0.036*
C2	0.9554 (3)	0.7565 (6)	−0.2695 (2)	0.0337 (11)
H2	0.9245 (3)	0.7281 (6)	−0.3049 (2)	0.040*
C3	0.9860 (3)	0.9523 (6)	−0.2739 (2)	0.0433 (13)
H3A	1.0030 (3)	0.9764 (6)	−0.3113 (2)	0.052*
H3B	1.0290 (3)	0.9717 (6)	−0.2452 (2)	0.052*
C4	0.9183 (3)	1.0790 (6)	−0.2616 (2)	0.0441 (13)
H4A	0.8970 (3)	1.1363 (6)	−0.2967 (2)	0.053*
H4B	0.9345 (3)	1.1728 (6)	−0.2341 (2)	0.053*
C5	0.8575 (3)	0.9539 (6)	−0.2372 (2)	0.0422 (12)
H5A	0.8370 (3)	1.0086 (6)	−0.2042 (2)	0.051*
H5B	0.8151 (3)	0.9299 (6)	−0.2660 (2)	0.051*
C6	0.8458 (2)	0.6152 (6)	−0.2133 (2)	0.0288 (10)
C7	0.8279 (2)	0.5558 (6)	−0.1591 (2)	0.0321 (11)
C8	0.7765 (3)	0.4133 (7)	−0.1524 (2)	0.0422 (12)
H8	0.7665 (3)	0.3760 (7)	−0.1142 (2)	0.051*
C9	0.7401 (3)	0.3271 (7)	−0.1997 (2)	0.0440 (13)
H9	0.7044 (3)	0.2284 (7)	−0.1950 (2)	0.053*
C10	0.7550 (3)	0.3838 (7)	−0.2538 (2)	0.0408 (12)
H10	0.7294 (3)	0.3248 (7)	−0.2873 (2)	0.049*
C11	0.8077 (3)	0.5225 (7)	−0.2605 (2)	0.0392 (12)
H11	0.8185 (3)	0.5592 (7)	−0.2986 (2)	0.047*
O12	0.8655 (2)	0.6379 (4)	−0.10890 (10)	0.0339 (8)
C13	0.8310 (3)	0.7883 (7)	−0.0882 (2)	0.0343 (11)
O14	0.7703 (2)	0.8507 (5)	−0.10761 (12)	0.0452 (9)
C15	0.8835 (2)	0.8682 (7)	−0.0378 (2)	0.0371 (12)
H15	0.8986 (2)	0.7727 (7)	−0.0106 (2)	0.045*
C16	0.9554 (3)	0.9465 (7)	−0.0617 (2)	0.0350 (11)
C17	0.9514 (3)	1.1159 (8)	−0.0889 (2)	0.0456 (13)
H17	0.9039 (3)	1.1847 (8)	−0.0898 (2)	0.055*

C18	1.0157 (3)	1.1819 (8)	−0.1147 (2)	0.056 (2)
H18	1.0141 (3)	1.2999 (8)	−0.1331 (2)	0.067*
C19	1.0830 (3)	1.0770 (8)	−0.1135 (2)	0.054 (2)
H19	1.1272 (3)	1.1209 (8)	−0.1317 (2)	0.065*
C20	1.0867 (3)	0.9108 (8)	−0.0856 (2)	0.0537 (15)
H20	1.1338 (3)	0.8401 (8)	−0.0851 (2)	0.064*
C21	1.0230 (3)	0.8458 (8)	−0.0594 (2)	0.0454 (13)
H21	1.0257 (3)	0.7312 (8)	−0.0391 (2)	0.054*
O22	0.8458 (2)	1.0083 (5)	−0.00957 (11)	0.0463 (9)
C23	0.7901 (3)	0.9421 (7)	0.0278 (2)	0.0507 (14)
H23A	0.7663 (3)	1.0438 (7)	0.0456 (2)	0.076*
H23B	0.7507 (3)	0.8719 (7)	0.0058 (2)	0.076*
H23C	0.8162 (3)	0.8658 (7)	0.0572 (2)	0.076*
C24	1.0184 (2)	0.6137 (6)	−0.2608 (2)	0.0273 (10)
C25	1.0375 (2)	0.4970 (6)	−0.30420 (15)	0.0271 (10)
C26	1.0982 (2)	0.3728 (6)	−0.2972 (2)	0.0335 (11)
H26	1.1101 (2)	0.2957 (6)	−0.3287 (2)	0.040*
C27	1.1427 (2)	0.3641 (7)	−0.2449 (2)	0.0375 (11)
H27	1.1843 (2)	0.2767 (7)	−0.2389 (2)	0.045*
C28	1.1257 (3)	0.4785 (7)	−0.2002 (2)	0.0363 (12)
H28	1.1574 (3)	0.4761 (7)	−0.1640 (2)	0.044*
C29	1.0648 (2)	0.6001 (7)	−0.2084 (2)	0.0342 (11)
H29	1.0521 (2)	0.6767 (7)	−0.1770 (2)	0.041*
O30	0.99019 (15)	0.4955 (4)	−0.35746 (10)	0.0316 (7)
C31	1.0136 (3)	0.5984 (7)	−0.4016 (2)	0.0309 (11)
O32	1.0738 (2)	0.6805 (5)	−0.39964 (12)	0.0482 (9)
C33	0.9501 (2)	0.5938 (7)	−0.45110 (15)	0.0311 (11)
H33	0.9333 (2)	0.4696 (7)	−0.45821 (15)	0.037*
C34	0.8823 (3)	0.7094 (7)	−0.4344 (2)	0.0325 (11)
C35	0.8908 (3)	0.8971 (7)	−0.4297 (2)	0.0379 (12)
H35	0.9381 (3)	0.9541 (7)	−0.4394 (2)	0.046*
C36	0.8311 (3)	1.0058 (7)	−0.4118 (2)	0.0447 (13)
H36	0.8372 (3)	1.1363 (7)	−0.4084 (2)	0.054*
C37	0.7626 (3)	0.9265 (8)	−0.3983 (2)	0.0444 (13)
H37	0.7219 (3)	0.9985 (8)	−0.3839 (2)	0.053*
C38	0.7528 (3)	0.7376 (8)	−0.4042 (2)	0.0399 (13)
H38	0.7042 (3)	0.6819 (8)	−0.3970 (2)	0.048*
C39	0.8125 (2)	0.6308 (7)	−0.4223 (2)	0.0362 (11)
H39	0.8053 (2)	0.5009 (7)	−0.4266 (2)	0.043*
O40	0.9827 (2)	0.6637 (5)	−0.50028 (11)	0.0389 (8)
C41	0.9291 (3)	0.6494 (8)	−0.5508 (2)	0.0507 (14)
H41A	0.9517 (3)	0.7012 (8)	−0.5833 (2)	0.076*
H41B	0.9170 (3)	0.5226 (8)	−0.5582 (2)	0.076*
H41C	0.8823 (3)	0.7146 (8)	−0.5444 (2)	0.076*
C1'	0.5959 (2)	0.7362 (6)	0.2267 (2)	0.0306 (11)
H1'	0.5744 (2)	0.6834 (6)	0.1909 (2)	0.037*
C2'	0.5278 (2)	0.7690 (6)	0.2641 (2)	0.0300 (11)
H2'	0.5495 (2)	0.8120 (6)	0.3012 (2)	0.036*
C3'	0.4843 (3)	0.9282 (7)	0.2329 (2)	0.0425 (12)

H3'A	0.4534 (3)	0.9956 (7)	0.2580 (2)	0.051*
H3'B	0.4507 (3)	0.8804 (7)	0.2011 (2)	0.051*
C4'	0.5478 (3)	1.0491 (7)	0.2104 (2)	0.0488 (14)
H4'A	0.5544 (3)	1.1582 (7)	0.2335 (2)	0.059*
H4'B	0.5343 (3)	1.0839 (7)	0.1709 (2)	0.059*
C5'	0.6222 (3)	0.9336 (7)	0.2150 (2)	0.0412 (12)
H5'A	0.6482 (3)	0.9407 (7)	0.1802 (2)	0.049*
H5'B	0.6572 (3)	0.9751 (7)	0.2468 (2)	0.049*
C6'	0.6603 (2)	0.6143 (6)	0.2530 (2)	0.0268 (10)
C7'	0.6917 (2)	0.4735 (6)	0.2223 (2)	0.0279 (10)
C8'	0.7541 (2)	0.3689 (7)	0.2443 (2)	0.0384 (12)
H8'	0.7738 (2)	0.2741 (7)	0.2209 (2)	0.046*
C9'	0.7871 (2)	0.4016 (7)	0.3001 (2)	0.0440 (13)
H9'	0.8310 (2)	0.3306 (7)	0.3158 (2)	0.053*
C10'	0.7568 (3)	0.5373 (7)	0.3325 (2)	0.0420 (13)
H10'	0.7791 (3)	0.5610 (7)	0.3711 (2)	0.050*
C11'	0.6943 (2)	0.6418 (7)	0.3090 (2)	0.0355 (11)
H11'	0.6726 (2)	0.7360 (7)	0.3316 (2)	0.043*
O12'	0.65765 (15)	0.4267 (4)	0.16644 (10)	0.0307 (7)
C13'	0.6744 (3)	0.5348 (7)	0.1213 (2)	0.0327 (11)
O14'	0.7186 (2)	0.6598 (5)	0.12533 (11)	0.0403 (8)
C15'	0.6270 (2)	0.4671 (6)	0.0670 (2)	0.0342 (11)
H15'	0.6328 (2)	0.3368 (6)	0.0635 (2)	0.041*
C16'	0.5415 (3)	0.5096 (7)	0.0693 (2)	0.0332 (11)
C17'	0.4871 (3)	0.3712 (7)	0.0704 (2)	0.0384 (12)
H17'	0.5039 (3)	0.2459 (7)	0.0688 (2)	0.046*
C18'	0.4095 (3)	0.4136 (8)	0.0732 (2)	0.0457 (14)
H18'	0.3720 (3)	0.3163 (8)	0.0734 (2)	0.055*
C19'	0.3859 (3)	0.5907 (9)	0.0749 (2)	0.0486 (14)
H19'	0.3318 (3)	0.6167 (9)	0.0778 (2)	0.058*
C20'	0.4387 (3)	0.7327 (8)	0.0724 (2)	0.0461 (13)
H20'	0.4202 (3)	0.8567 (8)	0.0733 (2)	0.055*
C21'	0.5172 (3)	0.6919 (7)	0.0707 (2)	0.0395 (13)
H21'	0.5546 (3)	0.7891 (7)	0.0697 (2)	0.047*
O22'	0.6519 (2)	0.5533 (5)	0.01741 (11)	0.0386 (8)
C23'	0.7247 (2)	0.4848 (8)	0.0023 (2)	0.0481 (14)
H23D	0.7397 (2)	0.5492 (8)	−0.0310 (2)	0.072*
H23E	0.7634 (2)	0.5040 (8)	0.0342 (2)	0.072*
H23F	0.7206 (2)	0.3562 (8)	−0.0062 (2)	0.072*
C24'	0.4769 (2)	0.6037 (6)	0.2734 (2)	0.0280 (10)
C25'	0.4599 (2)	0.5498 (6)	0.3277 (2)	0.0290 (10)
C26'	0.4135 (2)	0.3994 (6)	0.3366 (2)	0.0362 (12)
H26'	0.4066 (2)	0.3624 (6)	0.3754 (2)	0.043*
C27'	0.3795 (2)	0.3057 (7)	0.2898 (2)	0.0402 (12)
H27'	0.3460 (2)	0.2034 (7)	0.2955 (2)	0.048*
C28'	0.3927 (2)	0.3590 (6)	0.2344 (2)	0.0357 (11)
H28'	0.3677 (2)	0.2970 (6)	0.2013 (2)	0.043*
C29'	0.4419 (2)	0.5028 (6)	0.2269 (2)	0.0325 (11)
H29'	0.4532 (2)	0.5374 (6)	0.1887 (2)	0.039*

O30'	0.49177 (15)	0.6459 (4)	0.37721 (10)	0.0296 (7)
C31'	0.4488 (3)	0.7888 (6)	0.3942 (2)	0.0330 (11)
O32'	0.3870 (2)	0.8329 (5)	0.37064 (13)	0.0511 (9)
C33'	0.4909 (2)	0.8779 (6)	0.4471 (2)	0.0331 (11)
H33'	0.5024 (2)	0.7861 (6)	0.4762 (2)	0.040*
C34'	0.5658 (2)	0.9654 (6)	0.4318 (2)	0.0320 (11)
C35'	0.6345 (3)	0.9252 (7)	0.4647 (2)	0.0384 (11)
H35'	0.6325 (3)	0.8453 (7)	0.4974 (2)	0.046*
C36'	0.7048 (3)	0.9952 (7)	0.4499 (2)	0.0480 (13)
H36'	0.7520 (3)	0.9653 (7)	0.4732 (2)	0.058*
C37'	0.7061 (3)	1.1090 (7)	0.4029 (2)	0.0451 (13)
H37'	0.7547 (3)	1.1590 (7)	0.3930 (2)	0.054*
C38'	0.6381 (3)	1.1533 (7)	0.3704 (2)	0.0442 (13)
H38'	0.6389 (3)	1.2316 (7)	0.3373 (2)	0.053*
C39'	0.5678 (3)	1.0822 (6)	0.3846 (2)	0.0356 (11)
H39'	0.5198 (3)	1.1130 (6)	0.3624 (2)	0.043*
O40'	0.4422 (2)	1.0152 (4)	0.46907 (11)	0.0390 (8)
C41'	0.3839 (3)	0.9352 (7)	0.5016 (2)	0.0527 (14)
H41D	0.3521 (3)	1.0314 (7)	0.5150 (2)	0.079*
H41E	0.3521 (3)	0.8542 (7)	0.4769 (2)	0.079*
H41F	0.4076 (3)	0.8677 (7)	0.5340 (2)	0.079*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.031 (3)	0.031 (3)	0.027 (2)	0.008 (2)	0.001 (2)	0.000 (2)
C2	0.039 (3)	0.033 (3)	0.030 (2)	0.011 (2)	0.007 (2)	0.004 (2)
C3	0.058 (3)	0.034 (3)	0.041 (2)	0.005 (3)	0.020 (2)	0.008 (2)
C4	0.062 (3)	0.028 (3)	0.044 (2)	0.011 (3)	0.013 (2)	0.006 (2)
C5	0.053 (3)	0.030 (3)	0.046 (3)	0.013 (3)	0.018 (2)	0.007 (2)
C6	0.025 (2)	0.026 (2)	0.036 (2)	0.007 (2)	0.005 (2)	0.001 (2)
C7	0.026 (2)	0.037 (3)	0.034 (2)	0.003 (2)	0.004 (2)	−0.002 (2)
C8	0.040 (3)	0.039 (3)	0.049 (3)	0.000 (3)	0.014 (2)	−0.007 (3)
C9	0.032 (3)	0.034 (3)	0.067 (3)	−0.003 (3)	0.011 (3)	−0.014 (3)
C10	0.034 (3)	0.040 (3)	0.046 (3)	0.005 (3)	−0.007 (2)	−0.010 (3)
C11	0.041 (3)	0.038 (3)	0.038 (2)	0.006 (3)	0.001 (2)	−0.001 (2)
O12	0.036 (2)	0.037 (2)	0.0283 (14)	−0.003 (2)	0.0017 (14)	−0.0037 (15)
C13	0.042 (3)	0.035 (3)	0.027 (2)	−0.004 (3)	0.011 (2)	0.004 (2)
O14	0.040 (2)	0.053 (2)	0.043 (2)	0.007 (2)	0.003 (2)	−0.006 (2)
C15	0.047 (3)	0.035 (3)	0.029 (2)	0.001 (3)	0.003 (2)	0.001 (2)
C16	0.042 (3)	0.037 (3)	0.024 (2)	−0.005 (3)	−0.003 (2)	0.002 (2)
C17	0.039 (3)	0.051 (3)	0.045 (3)	−0.009 (3)	−0.003 (2)	0.014 (3)
C18	0.058 (4)	0.058 (4)	0.051 (3)	−0.017 (3)	0.000 (3)	0.012 (3)
C19	0.039 (3)	0.068 (4)	0.054 (3)	−0.015 (3)	0.002 (3)	−0.012 (3)
C20	0.040 (3)	0.058 (4)	0.061 (3)	−0.004 (3)	−0.002 (3)	−0.019 (3)
C21	0.049 (3)	0.042 (3)	0.044 (3)	−0.004 (3)	−0.004 (2)	−0.006 (3)
O22	0.065 (2)	0.038 (2)	0.039 (2)	−0.004 (2)	0.018 (2)	−0.006 (2)
C23	0.059 (3)	0.056 (4)	0.040 (2)	0.002 (3)	0.021 (2)	0.000 (3)

C24	0.029 (2)	0.027 (2)	0.026 (2)	0.000 (2)	0.008 (2)	0.002 (2)
C25	0.025 (2)	0.030 (3)	0.025 (2)	0.000 (2)	−0.002 (2)	0.002 (2)
C26	0.036 (3)	0.036 (3)	0.028 (2)	0.008 (2)	0.002 (2)	−0.006 (2)
C27	0.031 (3)	0.041 (3)	0.040 (2)	0.009 (2)	−0.001 (2)	0.002 (2)
C28	0.037 (3)	0.042 (3)	0.029 (2)	−0.001 (3)	−0.002 (2)	0.002 (2)
C29	0.040 (3)	0.035 (3)	0.027 (2)	0.005 (3)	0.002 (2)	−0.003 (2)
O30	0.028 (2)	0.043 (2)	0.0229 (13)	0.004 (2)	−0.0027 (12)	0.0021 (15)
C31	0.026 (3)	0.034 (3)	0.032 (2)	0.011 (2)	−0.001 (2)	−0.004 (2)
O32	0.031 (2)	0.068 (3)	0.044 (2)	−0.013 (2)	−0.006 (2)	0.018 (2)
C33	0.029 (2)	0.038 (3)	0.026 (2)	0.000 (2)	0.000 (2)	−0.001 (2)
C34	0.027 (3)	0.045 (3)	0.025 (2)	0.000 (2)	0.000 (2)	0.001 (2)
C35	0.027 (3)	0.042 (3)	0.046 (3)	−0.002 (3)	0.005 (2)	0.004 (2)
C36	0.047 (3)	0.036 (3)	0.051 (3)	0.003 (3)	0.003 (2)	0.001 (3)
C37	0.040 (3)	0.053 (4)	0.040 (3)	0.011 (3)	0.003 (2)	0.005 (3)
C38	0.021 (3)	0.057 (4)	0.042 (3)	0.001 (3)	0.005 (2)	0.009 (3)
C39	0.038 (3)	0.037 (3)	0.033 (2)	0.005 (3)	−0.001 (2)	0.005 (2)
O40	0.038 (2)	0.053 (2)	0.0267 (13)	0.008 (2)	0.0055 (14)	0.005 (2)
C41	0.053 (3)	0.070 (4)	0.027 (2)	0.013 (3)	−0.005 (2)	0.007 (3)
C1'	0.031 (3)	0.035 (3)	0.025 (2)	0.002 (2)	−0.001 (2)	0.002 (2)
C2'	0.034 (3)	0.027 (3)	0.030 (2)	0.001 (2)	0.006 (2)	0.002 (2)
C3'	0.043 (3)	0.036 (3)	0.051 (3)	0.007 (3)	0.010 (2)	0.001 (3)
C4'	0.055 (3)	0.033 (3)	0.060 (3)	0.005 (3)	0.012 (3)	0.016 (3)
C5'	0.044 (3)	0.037 (3)	0.044 (3)	0.000 (3)	0.007 (2)	0.009 (2)
C6'	0.025 (2)	0.027 (2)	0.029 (2)	−0.007 (2)	0.004 (2)	0.006 (2)
C7'	0.020 (2)	0.031 (3)	0.032 (2)	−0.004 (2)	0.002 (2)	0.006 (2)
C8'	0.031 (3)	0.038 (3)	0.047 (3)	0.007 (3)	0.007 (2)	0.015 (2)
C9'	0.024 (3)	0.055 (4)	0.052 (3)	0.002 (3)	−0.002 (2)	0.029 (3)
C10'	0.033 (3)	0.056 (4)	0.036 (2)	−0.013 (3)	−0.007 (2)	0.011 (3)
C11'	0.037 (3)	0.035 (3)	0.034 (2)	−0.004 (2)	0.002 (2)	0.000 (2)
O12'	0.032 (2)	0.033 (2)	0.0268 (14)	−0.005 (2)	0.0035 (13)	0.0006 (14)
C13'	0.033 (3)	0.032 (3)	0.034 (2)	0.004 (3)	0.010 (2)	−0.003 (2)
O14'	0.041 (2)	0.047 (2)	0.033 (2)	−0.017 (2)	0.0043 (15)	0.002 (2)
C15'	0.038 (3)	0.035 (3)	0.030 (2)	−0.009 (2)	0.008 (2)	−0.001 (2)
C16'	0.035 (3)	0.043 (3)	0.021 (2)	−0.007 (3)	−0.001 (2)	0.000 (2)
C17'	0.037 (3)	0.043 (3)	0.035 (2)	−0.004 (3)	0.001 (2)	−0.004 (2)
C18'	0.033 (3)	0.063 (4)	0.041 (3)	−0.017 (3)	−0.002 (2)	−0.003 (3)
C19'	0.032 (3)	0.079 (5)	0.032 (2)	0.001 (3)	−0.009 (2)	−0.001 (3)
C20'	0.044 (3)	0.051 (3)	0.042 (3)	0.011 (3)	−0.003 (2)	0.006 (3)
C21'	0.040 (3)	0.043 (3)	0.034 (2)	−0.013 (3)	−0.003 (2)	0.003 (2)
O22'	0.037 (2)	0.048 (2)	0.0317 (15)	−0.001 (2)	0.0087 (14)	0.0052 (15)
C23'	0.046 (3)	0.059 (4)	0.042 (2)	−0.009 (3)	0.020 (2)	−0.006 (3)
C24'	0.024 (2)	0.025 (2)	0.035 (2)	0.006 (2)	0.002 (2)	−0.002 (2)
C25'	0.026 (3)	0.027 (3)	0.034 (2)	0.003 (2)	0.001 (2)	−0.002 (2)
C26'	0.038 (3)	0.032 (3)	0.040 (2)	0.000 (2)	0.012 (2)	−0.003 (2)
C27'	0.028 (3)	0.032 (3)	0.061 (3)	−0.003 (2)	0.011 (2)	−0.009 (3)
C28'	0.033 (3)	0.031 (3)	0.042 (3)	0.003 (2)	−0.002 (2)	−0.017 (2)
C29'	0.033 (3)	0.032 (3)	0.032 (2)	0.005 (2)	0.002 (2)	−0.006 (2)
O30'	0.028 (2)	0.030 (2)	0.0300 (14)	0.000 (2)	0.0010 (13)	−0.0043 (14)
C31'	0.036 (3)	0.026 (3)	0.038 (2)	0.001 (2)	0.008 (2)	0.003 (2)

O32'	0.044 (2)	0.053 (2)	0.052 (2)	0.019 (2)	−0.016 (2)	−0.019 (2)
C33'	0.043 (3)	0.027 (3)	0.030 (2)	−0.004 (2)	0.003 (2)	0.002 (2)
C34'	0.041 (3)	0.027 (3)	0.028 (2)	−0.002 (2)	0.000 (2)	−0.002 (2)
C35'	0.044 (3)	0.032 (3)	0.037 (2)	−0.001 (3)	−0.005 (2)	0.007 (2)
C36'	0.042 (3)	0.048 (3)	0.052 (3)	0.000 (3)	−0.004 (2)	0.006 (3)
C37'	0.040 (3)	0.046 (3)	0.050 (3)	−0.012 (3)	0.004 (3)	−0.002 (3)
C38'	0.062 (3)	0.037 (3)	0.034 (2)	−0.014 (3)	0.008 (3)	0.000 (2)
C39'	0.040 (3)	0.035 (3)	0.031 (2)	0.000 (3)	−0.003 (2)	0.002 (2)
O40'	0.050 (2)	0.027 (2)	0.043 (2)	−0.003 (2)	0.016 (2)	−0.002 (2)
C41'	0.067 (4)	0.040 (3)	0.055 (3)	−0.001 (3)	0.026 (3)	0.006 (3)

Geometric parameters (Å, °)

C1—C6	1.504 (6)	C1'—C6'	1.507 (6)
C1—C5	1.540 (6)	C1'—C2'	1.540 (5)
C1—C2	1.547 (5)	C1'—C5'	1.541 (6)
C1—H1	0.96	C1'—H1'	0.96
C2—C24	1.504 (6)	C2'—C24'	1.519 (6)
C2—C3	1.529 (6)	C2'—C3'	1.528 (6)
C2—H2	0.96	C2'—H2'	0.96
C3—C4	1.536 (6)	C3'—C4'	1.534 (6)
C3—H3A	0.96	C3'—H3'A	0.96
C3—H3B	0.96	C3'—H3'B	0.96
C4—C5	1.537 (6)	C4'—C5'	1.530 (6)
C4—H4A	0.96	C4'—H4'A	0.96
C4—H4B	0.96	C4'—H4'B	0.96
C5—H5A	0.96	C5'—H5'A	0.96
C5—H5B	0.96	C5'—H5'B	0.96
C6—C7	1.392 (5)	C6'—C7'	1.389 (5)
C6—C11	1.400 (6)	C6'—C11'	1.392 (5)
C7—C8	1.383 (6)	C7'—C8'	1.378 (5)
C7—O12	1.415 (5)	C7'—O12'	1.416 (4)
C8—C9	1.366 (6)	C8'—C9'	1.389 (6)
C8—H8	0.96	C8'—H8'	0.96
C9—C10	1.372 (6)	C9'—C10'	1.375 (6)
C9—H9	0.96	C9'—H9'	0.96
C10—C11	1.378 (6)	C10'—C11'	1.389 (6)
C10—H10	0.96	C10'—H10'	0.96
C11—H11	0.96	C11'—H11'	0.96
O12—C13	1.357 (5)	O12'—C13'	1.364 (5)
C13—O14	1.191 (5)	C13'—O14'	1.186 (5)
C13—C15	1.528 (6)	C13'—C15'	1.522 (6)
C15—O22	1.405 (5)	C15'—O22'	1.413 (4)
C15—C16	1.516 (6)	C15'—C16'	1.511 (6)
C15—H15	0.96	C15'—H15'	0.96
C16—C21	1.373 (6)	C16'—C17'	1.380 (6)
C16—C17	1.386 (6)	C16'—C21'	1.396 (7)
C17—C18	1.394 (6)	C17'—C18'	1.380 (6)
C17—H17	0.96	C17'—H17'	0.96

C18—C19	1.388 (7)	C18'—C19'	1.356 (7)
C18—H18	0.96	C18'—H18'	0.96
C19—C20	1.373 (7)	C19'—C20'	1.384 (7)
C19—H19	0.96	C19'—H19'	0.96
C20—C21	1.387 (6)	C20'—C21'	1.388 (6)
C20—H20	0.96	C20'—H20'	0.96
C21—H21	0.96	C21'—H21'	0.96
O22—C23	1.437 (4)	O22'—C23'	1.424 (5)
C23—H23A	0.96	C23'—H23D	0.96
C23—H23B	0.96	C23'—H23E	0.96
C23—H23C	0.96	C23'—H23F	0.96
C24—C25	1.382 (5)	C24'—C25'	1.379 (5)
C24—C29	1.399 (5)	C24'—C29'	1.397 (5)
C25—C26	1.383 (6)	C25'—C26'	1.384 (6)
C25—O30	1.418 (4)	C25'—O30'	1.414 (5)
C26—C27	1.377 (5)	C26'—C27'	1.370 (6)
C26—H26	0.96	C26'—H26'	0.96
C27—C28	1.385 (5)	C27'—C28'	1.383 (5)
C27—H27	0.96	C27'—H27'	0.96
C28—C29	1.374 (6)	C28'—C29'	1.371 (6)
C28—H28	0.96	C28'—H28'	0.96
C29—H29	0.96	C29'—H29'	0.96
O30—C31	1.361 (5)	O30'—C31'	1.358 (5)
C31—O32	1.196 (5)	C31'—O32'	1.196 (5)
C31—C33	1.514 (5)	C31'—C33'	1.516 (6)
C33—O40	1.414 (4)	C33'—O40'	1.430 (5)
C33—C34	1.520 (6)	C33'—C34'	1.512 (6)
C33—H33	0.96	C33'—H33'	0.96
C34—C35	1.380 (6)	C34'—C35'	1.380 (5)
C34—C39	1.385 (6)	C34'—C39'	1.391 (5)
C35—C36	1.392 (6)	C35'—C36'	1.386 (6)
C35—H35	0.96	C35'—H35'	0.96
C36—C37	1.377 (6)	C36'—C37'	1.375 (6)
C36—H36	0.96	C36'—H36'	0.96
C37—C38	1.393 (7)	C37'—C38'	1.372 (6)
C37—H37	0.96	C37'—H37'	0.96
C38—C39	1.386 (6)	C38'—C39'	1.386 (6)
C38—H38	0.96	C38'—H38'	0.96
C39—H39	0.96	C39'—H39'	0.96
O40—C41	1.428 (5)	O40'—C41'	1.436 (5)
C41—H41A	0.96	C41'—H41D	0.96
C41—H41B	0.96	C41'—H41E	0.96
C41—H41C	0.96	C41'—H41F	0.96
C6—C1—C5	113.4 (3)	C6'—C1'—C2'	115.7 (3)
C6—C1—C2	117.4 (4)	C6'—C1'—C5'	113.9 (4)
C5—C1—C2	101.6 (3)	C2'—C1'—C5'	101.9 (3)
C6—C1—H1	108.7 (2)	C6'—C1'—H1'	109.0 (2)
C5—C1—H1	107.4 (2)	C2'—C1'—H1'	107.4 (2)
C2—C1—H1	107.8 (2)	C5'—C1'—H1'	108.5 (2)

C24—C2—C3	114.0 (4)	C24'—C2'—C3'	113.9 (3)
C24—C2—C1	116.2 (3)	C24'—C2'—C1'	115.9 (3)
C3—C2—C1	102.4 (3)	C3'—C2'—C1'	102.5 (3)
C24—C2—H2	107.6 (2)	C24'—C2'—H2'	108.2 (2)
C3—C2—H2	108.2 (3)	C3'—C2'—H2'	108.2 (2)
C1—C2—H2	108.1 (2)	C1'—C2'—H2'	107.7 (2)
C2—C3—C4	106.1 (3)	C2'—C3'—C4'	105.3 (3)
C2—C3—H3A	111.5 (2)	C2'—C3'—H3'A	112.1 (2)
C4—C3—H3A	111.0 (2)	C4'—C3'—H3'A	111.4 (3)
C2—C3—H3B	109.9 (3)	C2'—C3'—H3'B	108.9 (2)
C4—C3—H3B	109.4 (3)	C4'—C3'—H3'B	110.2 (2)
H3A—C3—H3B	108.8	H3'A—C3'—H3'B	108.9
C3—C4—C5	105.5 (4)	C5'—C4'—C3'	106.2 (4)
C3—C4—H4A	110.0 (2)	C5'—C4'—H4'A	111.2 (3)
C5—C4—H4A	110.6 (2)	C3'—C4'—H4'A	109.9 (3)
C3—C4—H4B	112.0 (3)	C5'—C4'—H4'B	109.8 (2)
C5—C4—H4B	110.1 (2)	C3'—C4'—H4'B	111.1 (2)
H4A—C4—H4B	108.7	H4'A—C4'—H4'B	108.7
C4—C5—C1	105.8 (3)	C4'—C5'—C1'	105.5 (3)
C4—C5—H5A	111.2 (2)	C4'—C5'—H5'A	111.4 (2)
C1—C5—H5A	111.3 (2)	C1'—C5'—H5'A	111.6 (2)
C4—C5—H5B	110.6 (2)	C4'—C5'—H5'B	110.0 (3)
C1—C5—H5B	109.2 (2)	C1'—C5'—H5'B	109.4 (2)
H5A—C5—H5B	108.8	H5'A—C5'—H5'B	108.9
C7—C6—C11	115.6 (4)	C7'—C6'—C11'	115.9 (4)
C7—C6—C1	122.6 (4)	C7'—C6'—C1'	122.4 (3)
C11—C6—C1	121.8 (4)	C11'—C6'—C1'	121.7 (4)
C8—C7—C6	122.2 (4)	C8'—C7'—C6'	123.2 (4)
C8—C7—O12	118.4 (4)	C8'—C7'—O12'	116.7 (4)
C6—C7—O12	119.4 (4)	C6'—C7'—O12'	120.1 (4)
C9—C8—C7	120.5 (4)	C7'—C8'—C9'	119.3 (4)
C9—C8—H8	120.3 (3)	C7'—C8'—H8'	119.5 (3)
C7—C8—H8	119.2 (3)	C9'—C8'—H8'	121.1 (3)
C8—C9—C10	119.2 (5)	C10'—C9'—C8'	119.4 (4)
C8—C9—H9	120.4 (3)	C10'—C9'—H9'	120.4 (3)
C10—C9—H9	120.4 (3)	C8'—C9'—H9'	120.2 (3)
C9—C10—C11	120.3 (4)	C9'—C10'—C11'	120.1 (4)
C9—C10—H10	119.9 (3)	C9'—C10'—H10'	120.1 (3)
C11—C10—H10	119.8 (3)	C11'—C10'—H10'	119.8 (3)
C10—C11—C6	122.2 (4)	C10'—C11'—C6'	122.2 (4)
C10—C11—H11	119.5 (3)	C10'—C11'—H11'	120.4 (3)
C6—C11—H11	118.2 (3)	C6'—C11'—H11'	117.5 (3)
C13—O12—C7	116.9 (3)	C13'—O12'—C7'	117.8 (3)
O14—C13—O12	124.9 (4)	O14'—C13'—O12'	124.3 (4)
O14—C13—C15	125.6 (5)	O14'—C13'—C15'	127.3 (4)
O12—C13—C15	109.4 (4)	O12'—C13'—C15'	108.4 (4)
O22—C15—C16	109.0 (4)	O22'—C15'—C16'	107.9 (3)
O22—C15—C13	111.6 (4)	O22'—C15'—C13'	110.6 (3)
C16—C15—C13	107.9 (3)	C16'—C15'—C13'	110.7 (3)

O22—C15—H15	109.2 (2)	O22'—C15'—H15'	109.3 (2)
C16—C15—H15	109.6 (2)	C16'—C15'—H15'	108.3 (3)
C13—C15—H15	109.5 (3)	C13'—C15'—H15'	109.9 (2)
C21—C16—C17	120.0 (4)	C17'—C16'—C21'	119.4 (4)
C21—C16—C15	120.2 (4)	C17'—C16'—C15'	121.2 (4)
C17—C16—C15	119.7 (4)	C21'—C16'—C15'	119.5 (4)
C16—C17—C18	119.8 (5)	C16'—C17'—C18'	120.0 (5)
C16—C17—H17	118.8 (3)	C16'—C17'—H17'	119.2 (3)
C18—C17—H17	121.4 (3)	C18'—C17'—H17'	120.8 (3)
C19—C18—C17	119.8 (5)	C19'—C18'—C17'	120.6 (5)
C19—C18—H18	119.6 (3)	C19'—C18'—H18'	120.1 (3)
C17—C18—H18	120.6 (3)	C17'—C18'—H18'	119.3 (3)
C20—C19—C18	119.9 (5)	C18'—C19'—C20'	120.7 (5)
C20—C19—H19	119.9 (3)	C18'—C19'—H19'	119.1 (3)
C18—C19—H19	120.2 (3)	C20'—C19'—H19'	120.2 (3)
C19—C20—C21	120.3 (5)	C19'—C20'—C21'	119.2 (5)
C19—C20—H20	118.8 (3)	C19'—C20'—H20'	118.9 (3)
C21—C20—H20	120.8 (3)	C21'—C20'—H20'	121.9 (3)
C16—C21—C20	120.2 (5)	C20'—C21'—C16'	120.0 (5)
C16—C21—H21	119.2 (3)	C20'—C21'—H21'	120.0 (3)
C20—C21—H21	120.6 (3)	C16'—C21'—H21'	120.0 (3)
C15—O22—C23	113.6 (4)	C15'—O22'—C23'	112.7 (3)
O22—C23—H23A	109.7 (2)	O22'—C23'—H23D	109.5 (2)
O22—C23—H23B	109.6 (2)	O22'—C23'—H23E	108.8 (2)
H23A—C23—H23B	109.5	H23D—C23'—H23E	109.5
O22—C23—H23C	109.2 (2)	O22'—C23'—H23F	110.0 (2)
H23A—C23—H23C	109.5	H23D—C23'—H23F	109.5
H23B—C23—H23C	109.5	H23E—C23'—H23F	109.5
C25—C24—C29	115.9 (4)	C25'—C24'—C29'	116.5 (4)
C25—C24—C2	123.1 (4)	C25'—C24'—C2'	122.0 (4)
C29—C24—C2	120.9 (4)	C29'—C24'—C2'	121.5 (4)
C24—C25—C26	123.1 (4)	C24'—C25'—C26'	122.4 (4)
C24—C25—O30	119.0 (4)	C24'—C25'—O30'	120.3 (4)
C26—C25—O30	117.8 (4)	C26'—C25'—O30'	117.3 (3)
C27—C26—C25	119.2 (4)	C27'—C26'—C25'	119.3 (4)
C27—C26—H26	120.4 (3)	C27'—C26'—H26'	121.6 (3)
C25—C26—H26	120.4 (2)	C25'—C26'—H26'	119.1 (2)
C26—C27—C28	119.8 (4)	C26'—C27'—C28'	120.2 (4)
C26—C27—H27	120.5 (3)	C26'—C27'—H27'	119.8 (3)
C28—C27—H27	119.8 (3)	C28'—C27'—H27'	120.0 (3)
C29—C28—C27	119.7 (4)	C29'—C28'—C27'	119.4 (4)
C29—C28—H28	119.9 (2)	C29'—C28'—H28'	119.8 (3)
C27—C28—H28	120.4 (3)	C27'—C28'—H28'	120.8 (3)
C28—C29—C24	122.3 (4)	C28'—C29'—C24'	122.2 (4)
C28—C29—H29	119.7 (2)	C28'—C29'—H29'	119.9 (2)
C24—C29—H29	118.0 (2)	C24'—C29'—H29'	117.9 (2)
C31—O30—C25	117.8 (3)	C31'—O30'—C25'	115.8 (3)
O32—C31—O30	124.3 (4)	O32'—C31'—O30'	124.0 (4)
O32—C31—C33	127.1 (4)	O32'—C31'—C33'	126.6 (4)

O30—C31—C33	108.5 (4)	O30'—C31'—C33'	109.4 (4)
O40—C33—C31	107.1 (3)	O40'—C33'—C34'	109.3 (3)
O40—C33—C34	112.2 (4)	O40'—C33'—C31'	109.7 (3)
C31—C33—C34	108.1 (3)	C34'—C33'—C31'	110.2 (3)
O40—C33—H33	109.7 (2)	O40'—C33'—H33'	109.1 (2)
C31—C33—H33	109.7 (3)	C34'—C33'—H33'	109.5 (2)
C34—C33—H33	110.0 (3)	C31'—C33'—H33'	109.0 (2)
C35—C34—C39	118.9 (4)	C35'—C34'—C39'	119.1 (4)
C35—C34—C33	119.5 (4)	C35'—C34'—C33'	119.2 (4)
C39—C34—C33	121.6 (4)	C39'—C34'—C33'	121.8 (4)
C34—C35—C36	120.8 (5)	C34'—C35'—C36'	120.5 (4)
C34—C35—H35	119.8 (3)	C34'—C35'—H35'	118.4 (3)
C36—C35—H35	119.3 (3)	C36'—C35'—H35'	121.1 (3)
C37—C36—C35	120.1 (5)	C37'—C36'—C35'	119.9 (5)
C37—C36—H36	119.2 (3)	C37'—C36'—H36'	120.7 (3)
C35—C36—H36	120.7 (3)	C35'—C36'—H36'	119.4 (3)
C36—C37—C38	119.4 (5)	C38'—C37'—C36'	120.2 (4)
C36—C37—H37	121.2 (3)	C38'—C37'—H37'	119.9 (3)
C38—C37—H37	119.3 (3)	C36'—C37'—H37'	119.9 (3)
C39—C38—C37	120.0 (5)	C37'—C38'—C39'	120.2 (4)
C39—C38—H38	119.9 (3)	C37'—C38'—H38'	120.4 (3)
C37—C38—H38	120.1 (3)	C39'—C38'—H38'	119.4 (3)
C34—C39—C38	120.8 (5)	C38'—C39'—C34'	120.1 (4)
C34—C39—H39	119.5 (3)	C38'—C39'—H39'	120.9 (3)
C38—C39—H39	119.7 (3)	C34'—C39'—H39'	119.1 (3)
C33—O40—C41	111.3 (3)	C33'—O40'—C41'	111.4 (3)
O40—C41—H41A	110.0 (2)	O40'—C41'—H41D	108.8 (2)
O40—C41—H41B	109.4 (3)	O40'—C41'—H41E	108.9 (2)
H41A—C41—H41B	109.5	H41D—C41'—H41E	109.5
O40—C41—H41C	109.0 (2)	O40'—C41'—H41F	110.7 (2)
H41A—C41—H41C	109.5	H41D—C41'—H41F	109.5
H41B—C41—H41C	109.5	H41E—C41'—H41F	109.5
C6—C1—C2—C24	−67.9 (5)	C6'—C1'—C2'—C24'	−68.1 (5)
C5—C1—C2—C24	167.8 (4)	C5'—C1'—C2'—C24'	167.7 (4)
C6—C1—C2—C3	167.2 (4)	C6'—C1'—C2'—C3'	167.2 (4)
C5—C1—C2—C3	42.9 (4)	C5'—C1'—C2'—C3'	43.0 (4)
C24—C2—C3—C4	−161.0 (3)	C24'—C2'—C3'—C4'	−161.9 (3)
C1—C2—C3—C4	−34.6 (4)	C1'—C2'—C3'—C4'	−35.8 (4)
C2—C3—C4—C5	12.5 (5)	C2'—C3'—C4'—C5'	14.6 (5)
C3—C4—C5—C1	14.8 (5)	C3'—C4'—C5'—C1'	12.4 (5)
C6—C1—C5—C4	−162.7 (3)	C6'—C1'—C5'—C4'	−159.6 (4)
C2—C1—C5—C4	−35.8 (4)	C2'—C1'—C5'—C4'	−34.3 (4)
C5—C1—C6—C7	−99.9 (5)	C2'—C1'—C6'—C7'	133.7 (4)
C2—C1—C6—C7	142.0 (4)	C5'—C1'—C6'—C7'	−108.6 (4)
C5—C1—C6—C11	77.8 (5)	C2'—C1'—C6'—C11'	−49.3 (5)
C2—C1—C6—C11	−40.3 (6)	C5'—C1'—C6'—C11'	68.4 (5)
C11—C6—C7—C8	0.7 (6)	C11'—C6'—C7'—C8'	−1.7 (6)
C1—C6—C7—C8	178.5 (4)	C1'—C6'—C7'—C8'	175.4 (4)
C11—C6—C7—O12	178.0 (4)	C11'—C6'—C7'—O12'	175.6 (3)

C1—C6—C7—O12	−4.2 (6)	C1'—C6'—C7'—O12'	−7.2 (6)
C6—C7—C8—C9	−1.2 (7)	C6'—C7'—C8'—C9'	1.1 (6)
O12—C7—C8—C9	−178.5 (4)	O12'—C7'—C8'—C9'	−176.4 (4)
C7—C8—C9—C10	−0.1 (7)	C7'—C8'—C9'—C10'	0.3 (6)
C8—C9—C10—C11	1.8 (7)	C8'—C9'—C10'—C11'	−0.8 (6)
C9—C10—C11—C6	−2.4 (7)	C9'—C10'—C11'—C6'	0.1 (7)
C7—C6—C11—C10	1.1 (6)	C7'—C6'—C11'—C10'	1.1 (6)
C1—C6—C11—C10	−176.8 (4)	C1'—C6'—C11'—C10'	−176.0 (4)
C8—C7—O12—C13	−93.5 (5)	C8'—C7'—O12'—C13'	−103.4 (4)
C6—C7—O12—C13	89.1 (4)	C6'—C7'—O12'—C13'	79.1 (4)
C7—O12—C13—O14	3.3 (6)	C7'—O12'—C13'—O14'	4.0 (6)
C7—O12—C13—C15	−174.6 (3)	C7'—O12'—C13'—C15'	−175.9 (3)
O14—C13—C15—O22	10.4 (6)	O14'—C13'—C15'—O22'	10.3 (6)
O12—C13—C15—O22	−171.7 (3)	O12'—C13'—C15'—O22'	−169.9 (3)
O14—C13—C15—C16	−109.4 (5)	O14'—C13'—C15'—C16'	−109.4 (5)
O12—C13—C15—C16	68.6 (5)	O12'—C13'—C15'—C16'	70.5 (4)
O22—C15—C16—C21	140.9 (4)	O22'—C15'—C16'—C17'	122.6 (4)
C13—C15—C16—C21	−97.7 (5)	C13'—C15'—C16'—C17'	−116.2 (4)
O22—C15—C16—C17	−42.8 (5)	O22'—C15'—C16'—C21'	−57.7 (5)
C13—C15—C16—C17	78.6 (5)	C13'—C15'—C16'—C21'	63.5 (5)
C21—C16—C17—C18	1.1 (7)	C21'—C16'—C17'—C18'	−0.6 (6)
C15—C16—C17—C18	−175.2 (4)	C15'—C16'—C17'—C18'	179.1 (4)
C16—C17—C18—C19	0.6 (7)	C16'—C17'—C18'—C19'	0.2 (7)
C17—C18—C19—C20	−1.7 (8)	C17'—C18'—C19'—C20'	1.4 (7)
C18—C19—C20—C21	1.2 (7)	C18'—C19'—C20'—C21'	−2.6 (7)
C17—C16—C21—C20	−1.7 (7)	C19'—C20'—C21'—C16'	2.3 (7)
C15—C16—C21—C20	174.6 (4)	C17'—C16'—C21'—C20'	−0.7 (7)
C19—C20—C21—C16	0.5 (7)	C15'—C16'—C21'—C20'	179.6 (4)
C16—C15—O22—C23	−164.0 (3)	C16'—C15'—O22'—C23'	−164.5 (4)
C13—C15—O22—C23	76.9 (4)	C13'—C15'—O22'—C23'	74.3 (4)
C3—C2—C24—C25	−105.0 (5)	C3'—C2'—C24'—C25'	−112.8 (5)
C1—C2—C24—C25	136.2 (4)	C1'—C2'—C24'—C25'	128.6 (4)
C3—C2—C24—C29	70.7 (5)	C3'—C2'—C24'—C29'	64.5 (5)
C1—C2—C24—C29	−48.0 (6)	C1'—C2'—C24'—C29'	−54.2 (5)
C29—C24—C25—C26	0.2 (6)	C29'—C24'—C25'—C26'	2.6 (6)
C2—C24—C25—C26	176.2 (4)	C2'—C24'—C25'—C26'	180.0 (4)
C29—C24—C25—O30	176.4 (4)	C29'—C24'—C25'—O30'	−179.0 (4)
C2—C24—C25—O30	−7.7 (6)	C2'—C24'—C25'—O30'	−1.7 (6)
C24—C25—C26—C27	−0.4 (7)	C24'—C25'—C26'—C27'	−3.6 (6)
O30—C25—C26—C27	−176.6 (4)	O30'—C25'—C26'—C27'	178.0 (4)
C25—C26—C27—C28	0.3 (6)	C25'—C26'—C27'—C28'	1.3 (7)
C26—C27—C28—C29	−0.1 (7)	C26'—C27'—C28'—C29'	1.9 (7)
C27—C28—C29—C24	0.0 (7)	C27'—C28'—C29'—C24'	−2.9 (6)
C25—C24—C29—C28	0.0 (6)	C25'—C24'—C29'—C28'	0.7 (6)
C2—C24—C29—C28	−176.1 (4)	C2'—C24'—C29'—C28'	−176.7 (4)
C24—C25—O30—C31	96.7 (4)	C24'—C25'—O30'—C31'	89.6 (4)
C26—C25—O30—C31	−87.0 (5)	C26'—C25'—O30'—C31'	−92.0 (4)
C25—O30—C31—O32	5.1 (6)	C25'—O30'—C31'—O32'	1.4 (6)
C25—O30—C31—C33	−173.4 (3)	C25'—O30'—C31'—C33'	−179.5 (3)

O32—C31—C33—O40	15.1 (6)	O32'—C31'—C33'—O40'	5.5 (6)
O30—C31—C33—O40	−166.5 (3)	O30'—C31'—C33'—O40'	−173.6 (3)
O32—C31—C33—C34	−106.1 (5)	O32'—C31'—C33'—C34'	−114.8 (5)
O30—C31—C33—C34	72.4 (4)	O30'—C31'—C33'—C34'	66.1 (4)
O40—C33—C34—C35	−49.1 (5)	O40'—C33'—C34'—C35'	110.7 (4)
C31—C33—C34—C35	68.7 (5)	C31'—C33'—C34'—C35'	−128.7 (4)
O40—C33—C34—C39	132.4 (4)	O40'—C33'—C34'—C39'	−70.8 (5)
C31—C33—C34—C39	−109.7 (5)	C31'—C33'—C34'—C39'	49.8 (6)
C39—C34—C35—C36	1.5 (7)	C39'—C34'—C35'—C36'	−2.1 (7)
C33—C34—C35—C36	−177.0 (3)	C33'—C34'—C35'—C36'	176.5 (4)
C34—C35—C36—C37	0.4 (7)	C34'—C35'—C36'—C37'	1.4 (7)
C35—C36—C37—C38	−1.8 (7)	C35'—C36'—C37'—C38'	−0.1 (7)
C36—C37—C38—C39	1.4 (7)	C36'—C37'—C38'—C39'	−0.6 (7)
C35—C34—C39—C38	−1.9 (6)	C37'—C38'—C39'—C34'	−0.1 (7)
C33—C34—C39—C38	176.6 (4)	C35'—C34'—C39'—C38'	1.4 (6)
C37—C38—C39—C34	0.4 (7)	C33'—C34'—C39'—C38'	−177.1 (4)
C31—C33—O40—C41	174.7 (4)	C34'—C33'—O40'—C41'	−160.7 (3)
C34—C33—O40—C41	−66.8 (5)	C31'—C33'—O40'—C41'	78.4 (4)