Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Redetermination and H-atom refinement of (*S*)-(+)-ibuprofen. Corrigendum.

Lars Kr. Hansen,[a]* German L. Perlovich[b,c] and Annette Bauer-Brandl[b]

[a]Department of Chemistry, University of Tromsø, 9037 Tromsø, Norway, [b]Department of Pharmaceutics and Biopharmaceutics, University of Tromsø, 9037 Tromsø, Norway, and [c]Institute of Solution Chemistry, Russian Academy of Sciences, 153045 Ivanovo, Russian Federation

Correspondence e-mail: larsk@chem.uit.no

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.038
wR factor = 0.104
Data-to-parameter ratio = 7.0

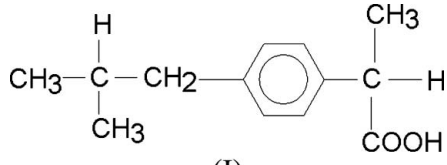
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 May 2006
Accepted 31 May 2006

In the paper by Hansen, Perlovich & Bauer-Brandl [*Acta Cryst.* (2003), E**59**, o1357–o1358], the coordinates of the *R* enantiomer of the title compound, $C_{13}H_{18}O_2$, were incorrectly given instead of those of the *S* enantiomer. The correct coordinates of the *S* enantiomer are given here.

Comment

In the paper by Hansen *et al.* (2003), the coordinates of the *R* enantiomer were incorrectly given instead of those of the *S* enantiomer, (I). The correct coordinates of the *S* enantiomer are given in the deposited replacement CIF. Molecular geometry parameters are not affected, except for the signs of torsion angles; the correct values are given in Table 1 below for the torsion angles in Table 2 of the previous report (where there was also an error in the atom numbering). Fig. 1 shows the correct structure of the two independent molecules, which form a hydrogen-bonded dimer without crystallographic symmetry.



(I)

Experimental

Table 1
Selected torsion angles (°).

C5*B*—C4*B*—C2*B*—C3*B*	29.1 (4)	O1*A*—C1*A*—C2*A*—C4*A*	−81.7 (4)
C7*B*—C10*B*—C11*B*—C12*B*	−68.0 (5)	C3*A*—C2*A*—C4*A*—C5*A*	−144.4 (4)
C4*B*—C2*B*—C1*B*—O1*B*	83.5 (3)	C7*A*—C10*A*—C11*A*—C13*A*	67.9 (5)

All H atoms were refined freely [C—H = 0.85 (3)–114 (5) Å].

Data collection: *CAD-4-PC* Software (Enraf–Nonius, 1992); cell refinement: *CELDIM* in *CAD-4-PC* Software; data reduction: *XCAD* (McArdle & Higgins, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *OSCAIL* (McArdle, 1993).

References

Enraf–Nonius (1992). *CAD-4-PC Software*. Enraf–Nonius, Delft, The Netherlands.

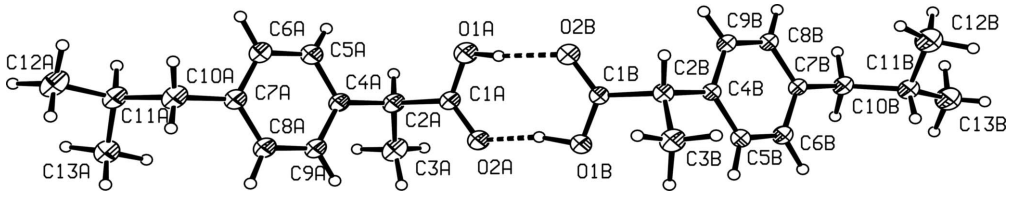


Figure 1
The structure of the two independent molecules of (I). Displacement ellipsoids are shown at the 30% probability level. Hydrogen bonds are shown as dashed lines.

Hansen, L. K., Perlovich, G. L. & Bauer-Brandl, A. (2003). *Acta Cryst.* E**59**, o1357–o1358.
McArdle, P. (1993). *J. Appl. Cryst.* **26**, 752.
McArdle, P. (1995). *J. Appl. Cryst.* **28**, 65.
McArdle, P. & Higgins, T. (1995). *XCAD*. NUI Galway, Ireland.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

supporting information

Acta Cryst. (2006). E**62**, e17–e18 [https://doi.org/10.1107/S1600536806020575]

Redetermination and H-atom refinement of (*S*)-(+)-ibuprofen. Corrigendum.

Lars Kr. Hansen, German L. Perlovich and Annette Bauer-Brandl

S(+)-2-(4-Isobutylphenyl)propionic acid

Crystal data

$C_{13}H_{18}O_2$
$M_r = 206.27$
Monoclinic, $P2_1$
$a = 12.456$ (4) Å
$b = 8.0362$ (11) Å
$c = 13.533$ (3) Å
$\beta = 112.86$ (2)°
$V = 1248.2$ (5) Å^3
$Z = 4$
$F(000) = 448$
$D_x = 1.098$ Mg m^{-3}
Melting point: 323.45 K
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 14$–20°
$\mu = 0.07$ mm^{-1}
$T = 298$ K
Block, colourless
0.40 × 0.40 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω–2θ scans
3086 measured reflections
2910 independent reflections
1683 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.6°$
$h = 0 \rightarrow 15$
$k = -1 \rightarrow 10$
$l = -17 \rightarrow 15$
3 standard reflections every 120 min
intensity decay: 2%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.104$
$S = 0.99$
2910 reflections
416 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.12$ e Å^{-3}
$\Delta\rho_{min} = -0.11$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.016 (3)

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C4B	0.1599 (2)	0.6802 (3)	0.9686 (2)	0.0497 (7)
O2A	0.41501 (19)	1.2352 (3)	1.10391 (18)	0.0757 (6)
O1A	0.5360 (2)	1.0661 (4)	1.2241 (2)	0.0890 (8)
O1B	0.2315 (2)	1.0390 (3)	1.04780 (18)	0.0710 (6)
O2B	0.3514 (2)	0.8687 (3)	1.16959 (17)	0.0840 (7)
C7B	0.1665 (2)	0.5002 (3)	0.7917 (2)	0.0493 (7)
C9B	0.2332 (2)	0.5454 (4)	0.9825 (2)	0.0547 (7)
C6B	0.0946 (3)	0.6374 (4)	0.7780 (2)	0.0604 (8)
C8B	0.2368 (2)	0.4578 (4)	0.8959 (2)	0.0548 (7)
C2B	0.1572 (3)	0.7722 (4)	1.0655 (2)	0.0590 (8)
C5B	0.0915 (3)	0.7254 (4)	0.8642 (2)	0.0599 (8)
C10B	0.1645 (3)	0.4036 (4)	0.6966 (2)	0.0614 (8)
C11B	0.0598 (3)	0.2872 (5)	0.6492 (2)	0.0689 (9)
C1B	0.2553 (3)	0.8986 (4)	1.0998 (2)	0.0547 (7)
C12B	0.0653 (5)	0.1455 (7)	0.7241 (4)	0.1069 (17)
C3B	0.0409 (3)	0.8537 (6)	1.0477 (4)	0.0835 (11)
C13B	0.0514 (6)	0.2219 (7)	0.5405 (4)	0.1046 (15)
H3B3	0.010 (3)	0.953 (6)	0.983 (3)	0.117 (14)*
H133	0.830 (4)	1.953 (8)	1.765 (4)	0.16 (2)*
H123	0.637 (5)	2.006 (10)	1.537 (4)	0.18 (3)*
H1BO	0.312 (4)	1.106 (6)	1.077 (3)	0.113 (13)*
H132	0.775 (4)	1.765 (7)	1.783 (4)	0.129 (18)*
H131	0.672 (4)	1.925 (7)	1.732 (4)	0.16 (2)*
H126	0.135 (6)	0.067 (12)	0.714 (6)	0.24 (3)*
H3B2	0.051 (2)	0.906 (4)	1.118 (2)	0.072 (9)*
H2B	0.179 (2)	0.691 (4)	1.128 (2)	0.064 (8)*
H3B1	−0.020 (4)	0.764 (8)	1.031 (4)	0.144 (18)*
H125	0.087 (4)	0.174 (6)	0.800 (4)	0.114 (14)*
H124	−0.015 (5)	0.083 (9)	0.690 (4)	0.16 (2)*
H103	0.160 (2)	0.487 (4)	0.640 (2)	0.068 (9)*
H104	0.239 (3)	0.335 (4)	0.721 (2)	0.065 (9)*
H6B	0.043 (3)	0.674 (4)	0.701 (3)	0.075 (9)*
H136	0.117 (4)	0.150 (7)	0.565 (4)	0.14 (2)*
H8B	0.288 (3)	0.368 (5)	0.907 (2)	0.073 (9)*
H134	−0.009 (3)	0.159 (5)	0.515 (3)	0.074 (11)*

H5B	0.034 (2)	0.817 (4)	0.848 (2)	0.071 (9)*
H9B	0.288 (3)	0.520 (5)	1.053 (3)	0.093 (11)*
H135	0.051 (5)	0.321 (10)	0.484 (5)	0.19 (3)*
H11B	−0.020 (3)	0.345 (4)	0.6456 (19)	0.065 (8)*
H3A3	0.668 (3)	1.522 (6)	1.127 (3)	0.108 (12)*
H11A	0.805 (4)	1.741 (6)	1.642 (3)	0.111 (14)*
H101	0.566 (3)	1.741 (5)	1.577 (3)	0.088 (12)*
H3A2	0.597 (3)	1.385 (6)	1.050 (3)	0.104 (14)*
H102	0.652 (3)	1.600 (6)	1.645 (3)	0.114 (15)*
H121	0.702 (3)	1.904 (6)	1.474 (3)	0.108 (12)*
H122	0.790 (4)	2.024 (7)	1.584 (3)	0.122 (14)*
H6A	0.743 (3)	1.404 (6)	1.563 (3)	0.105 (12)*
H2A	0.674 (3)	1.266 (5)	1.217 (3)	0.096 (12)*
H8A	0.500 (3)	1.738 (5)	1.377 (2)	0.074 (9)*
H9A	0.500 (3)	1.598 (4)	1.227 (2)	0.059 (8)*
H5A	0.729 (3)	1.283 (5)	1.398 (2)	0.074 (10)*
H1AO	0.466 (4)	1.007 (8)	1.208 (4)	0.16 (2)*
H3A1	0.519 (4)	1.503 (6)	1.073 (3)	0.132 (16)*
C1A	0.5121 (3)	1.2052 (4)	1.1705 (2)	0.0613 (8)
C2A	0.6101 (3)	1.3274 (4)	1.1995 (3)	0.0680 (9)
C3A	0.5972 (4)	1.4412 (7)	1.1044 (4)	0.0899 (13)
C4A	0.6163 (2)	1.4215 (4)	1.2990 (2)	0.0592 (8)
C5A	0.6865 (3)	1.3646 (5)	1.4000 (3)	0.0776 (10)
C6A	0.6905 (3)	1.4469 (5)	1.4913 (3)	0.0796 (10)
C7A	0.6248 (3)	1.5870 (4)	1.4856 (3)	0.0666 (9)
C8A	0.5540 (3)	1.6416 (5)	1.3850 (3)	0.0685 (9)
C9A	0.5499 (3)	1.5605 (4)	1.2941 (3)	0.0660 (8)
C10A	0.6351 (4)	1.6797 (6)	1.5864 (3)	0.0820 (12)
C11A	0.7349 (3)	1.8032 (5)	1.6258 (3)	0.0756 (10)
C13A	0.7144 (5)	1.9476 (6)	1.5496 (4)	0.0921 (13)
C12A	0.7559 (5)	1.8665 (9)	1.7376 (3)	0.1028 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C4B	0.0532 (14)	0.0418 (16)	0.0556 (16)	−0.0049 (13)	0.0229 (12)	−0.0050 (13)
O2A	0.0602 (12)	0.0612 (14)	0.0891 (14)	−0.0027 (11)	0.0106 (11)	0.0095 (12)
O1A	0.0719 (16)	0.0732 (17)	0.0998 (18)	0.0059 (14)	0.0094 (13)	0.0200 (15)
O1B	0.0699 (14)	0.0505 (13)	0.0826 (14)	0.0005 (11)	0.0186 (11)	0.0060 (12)
O2B	0.0822 (14)	0.0658 (15)	0.0800 (13)	−0.0033 (13)	0.0051 (13)	0.0127 (13)
C7B	0.0488 (14)	0.0476 (16)	0.0541 (16)	−0.0071 (13)	0.0227 (12)	−0.0038 (14)
C9B	0.0545 (16)	0.0520 (17)	0.0523 (16)	0.0047 (15)	0.0148 (13)	0.0004 (14)
C6B	0.0728 (19)	0.0565 (18)	0.0504 (17)	0.0013 (17)	0.0224 (15)	0.0047 (15)
C8B	0.0555 (16)	0.0487 (16)	0.0566 (16)	0.0090 (15)	0.0178 (13)	0.0005 (14)
C2B	0.0716 (19)	0.0511 (19)	0.0646 (18)	−0.0018 (16)	0.0379 (15)	−0.0023 (16)
C5B	0.0644 (17)	0.0455 (17)	0.0676 (19)	0.0141 (15)	0.0231 (15)	0.0061 (15)
C10B	0.0675 (19)	0.064 (2)	0.0547 (16)	−0.0061 (17)	0.0259 (14)	−0.0025 (17)
C11B	0.075 (2)	0.066 (2)	0.0639 (19)	−0.0088 (18)	0.0247 (16)	−0.0154 (17)

C1B	0.0708 (18)	0.0455 (17)	0.0530 (16)	0.0069 (15)	0.0296 (15)	−0.0022 (14)
C12B	0.137 (4)	0.098 (4)	0.086 (3)	−0.047 (3)	0.043 (3)	−0.009 (3)
C3B	0.079 (2)	0.080 (3)	0.111 (3)	−0.006 (2)	0.058 (2)	−0.028 (3)
C13B	0.134 (4)	0.093 (3)	0.077 (3)	−0.022 (4)	0.030 (3)	−0.030 (3)
C1A	0.0580 (18)	0.059 (2)	0.0647 (18)	0.0051 (16)	0.0210 (16)	−0.0113 (18)
C2A	0.0517 (17)	0.069 (2)	0.084 (2)	0.0060 (17)	0.0268 (16)	−0.0115 (19)
C3A	0.096 (3)	0.105 (3)	0.085 (3)	−0.027 (3)	0.053 (2)	−0.014 (3)
C4A	0.0421 (14)	0.059 (2)	0.0702 (19)	−0.0021 (14)	0.0149 (13)	−0.0007 (16)
C5A	0.076 (2)	0.059 (2)	0.087 (3)	0.014 (2)	0.0197 (19)	−0.003 (2)
C6A	0.089 (2)	0.069 (2)	0.064 (2)	0.002 (2)	0.0107 (18)	0.006 (2)
C7A	0.0706 (19)	0.063 (2)	0.069 (2)	−0.0111 (17)	0.0302 (16)	−0.0028 (18)
C8A	0.0582 (18)	0.068 (2)	0.073 (2)	0.0080 (18)	0.0184 (16)	−0.0084 (19)
C9A	0.0570 (17)	0.065 (2)	0.0634 (19)	0.0084 (17)	0.0098 (15)	−0.0041 (18)
C10A	0.089 (3)	0.093 (3)	0.071 (2)	−0.017 (2)	0.038 (2)	−0.006 (2)
C11A	0.073 (2)	0.086 (3)	0.0644 (19)	0.000 (2)	0.0234 (16)	−0.007 (2)
C13A	0.106 (3)	0.084 (3)	0.084 (3)	−0.013 (3)	0.036 (3)	−0.003 (2)
C12A	0.105 (3)	0.126 (4)	0.073 (2)	−0.010 (3)	0.030 (2)	−0.022 (3)

Geometric parameters (Å, º)

C4B—C9B	1.382 (4)	C13B—H136	0.95 (5)
C4B—C5B	1.385 (4)	C13B—H134	0.86 (4)
C4B—C2B	1.517 (4)	C13B—H135	1.10 (7)
O2A—C1A	1.219 (3)	C1A—C2A	1.496 (5)
O1A—C1A	1.303 (4)	C2A—C4A	1.519 (4)
O1A—H1AO	0.94 (6)	C2A—C3A	1.536 (6)
O1B—C1B	1.301 (4)	C2A—H2A	0.89 (4)
O1B—H1BO	1.07 (5)	C3A—H3A3	1.05 (4)
O2B—C1B	1.226 (3)	C3A—H3A2	0.87 (4)
C7B—C8B	1.383 (4)	C3A—H3A1	1.03 (5)
C7B—C6B	1.386 (4)	C4A—C9A	1.377 (4)
C7B—C10B	1.495 (4)	C4A—C5A	1.384 (4)
C9B—C8B	1.382 (4)	C5A—C6A	1.385 (5)
C9B—H9B	0.96 (3)	C5A—H5A	0.85 (3)
C6B—C5B	1.378 (4)	C6A—C7A	1.376 (5)
C6B—H6B	1.03 (3)	C6A—H6A	1.00 (4)
C8B—H8B	0.93 (4)	C7A—C8A	1.375 (4)
C2B—C1B	1.517 (4)	C7A—C10A	1.515 (5)
C2B—C3B	1.521 (5)	C8A—C9A	1.374 (4)
C2B—H2B	1.01 (3)	C8A—H8A	1.01 (4)
C5B—H5B	0.99 (3)	C9A—H9A	0.93 (3)
C10B—C11B	1.529 (4)	C10A—C11A	1.516 (6)
C10B—H103	1.00 (3)	C10A—H101	0.96 (4)
C10B—H104	1.01 (3)	C10A—H102	0.97 (5)
C11B—C12B	1.508 (6)	C11A—C13A	1.506 (6)
C11B—C13B	1.526 (5)	C11A—C12A	1.520 (5)
C11B—H11B	1.08 (3)	C11A—H11A	0.95 (4)
C12B—H126	1.12 (8)	C13A—H123	1.03 (6)

C12B—H125	0.98 (4)	C13A—H121	1.04 (4)
C12B—H124	1.05 (6)	C13A—H122	1.06 (5)
C3B—H3B3	1.14 (5)	C12A—H133	1.10 (6)
C3B—H3B2	1.00 (3)	C12A—H132	0.99 (6)
C3B—H3B1	1.00 (6)	C12A—H131	1.12 (5)
C9B—C4B—C5B	117.1 (3)	H134—C13B—H135	112 (4)
C9B—C4B—C2B	120.0 (3)	O2A—C1A—O1A	121.9 (3)
C5B—C4B—C2B	122.8 (3)	O2A—C1A—C2A	122.6 (3)
C1A—O1A—H1AO	108 (4)	O1A—C1A—C2A	115.5 (3)
C1B—O1B—H1BO	105 (2)	C1A—C2A—C4A	108.3 (3)
C8B—C7B—C6B	116.9 (3)	C1A—C2A—C3A	111.3 (3)
C8B—C7B—C10B	122.8 (3)	C4A—C2A—C3A	113.5 (3)
C6B—C7B—C10B	120.3 (3)	C1A—C2A—H2A	105 (3)
C8B—C9B—C4B	121.4 (3)	C4A—C2A—H2A	108 (2)
C8B—C9B—H9B	120 (2)	C3A—C2A—H2A	110 (2)
C4B—C9B—H9B	118 (2)	C2A—C3A—H3A3	109 (2)
C5B—C6B—C7B	121.7 (3)	C2A—C3A—H3A2	112 (3)
C5B—C6B—H6B	119.4 (19)	H3A3—C3A—H3A2	107 (3)
C7B—C6B—H6B	119.0 (19)	C2A—C3A—H3A1	114 (2)
C9B—C8B—C7B	121.5 (3)	H3A3—C3A—H3A1	113 (4)
C9B—C8B—H8B	119.7 (18)	H3A2—C3A—H3A1	103 (3)
C7B—C8B—H8B	118.7 (17)	C9A—C4A—C5A	116.9 (3)
C4B—C2B—C1B	107.7 (2)	C9A—C4A—C2A	122.6 (3)
C4B—C2B—C3B	114.4 (3)	C5A—C4A—C2A	120.4 (3)
C1B—C2B—C3B	111.4 (3)	C4A—C5A—C6A	120.9 (4)
C4B—C2B—H2B	108.2 (16)	C4A—C5A—H5A	113 (2)
C1B—C2B—H2B	104.6 (16)	C6A—C5A—H5A	126 (2)
C3B—C2B—H2B	110.0 (15)	C7A—C6A—C5A	121.7 (4)
C6B—C5B—C4B	121.3 (3)	C7A—C6A—H6A	119 (2)
C6B—C5B—H5B	116.7 (16)	C5A—C6A—H6A	119 (2)
C4B—C5B—H5B	121.8 (16)	C8A—C7A—C6A	117.1 (3)
C7B—C10B—C11B	113.9 (3)	C8A—C7A—C10A	122.2 (3)
C7B—C10B—H103	106.8 (17)	C6A—C7A—C10A	120.7 (4)
C11B—C10B—H103	107.5 (16)	C9A—C8A—C7A	121.4 (3)
C7B—C10B—H104	107.4 (16)	C9A—C8A—H8A	118.3 (17)
C11B—C10B—H104	109.0 (18)	C7A—C8A—H8A	120.2 (17)
H103—C10B—H104	112 (2)	C8A—C9A—C4A	121.9 (3)
C12B—C11B—C13B	110.9 (4)	C8A—C9A—H9A	120.0 (18)
C12B—C11B—C10B	111.8 (3)	C4A—C9A—H9A	118.0 (18)
C13B—C11B—C10B	110.0 (4)	C7A—C10A—C11A	114.2 (3)
C12B—C11B—H11B	98.8 (16)	C7A—C10A—H101	112 (2)
C13B—C11B—H11B	112.7 (14)	C11A—C10A—H101	106 (2)
C10B—C11B—H11B	112.2 (17)	C7A—C10A—H102	109 (3)
O2B—C1B—O1B	122.4 (3)	C11A—C10A—H102	105 (3)
O2B—C1B—C2B	122.2 (3)	H101—C10A—H102	111 (3)
O1B—C1B—C2B	115.3 (3)	C13A—C11A—C10A	111.5 (4)
C11B—C12B—H126	100 (4)	C13A—C11A—C12A	110.0 (4)

C11B—C12B—H125	117 (3)	C10A—C11A—C12A	111.7 (4)
H126—C12B—H125	110 (4)	C13A—C11A—H11A	117 (3)
C11B—C12B—H124	106 (3)	C10A—C11A—H11A	107 (3)
H126—C12B—H124	109 (5)	C12A—C11A—H11A	99 (2)
H125—C12B—H124	113 (4)	C11A—C13A—H123	112 (4)
C2B—C3B—H3B3	116 (2)	C11A—C13A—H121	110 (3)
C2B—C3B—H3B2	105.4 (17)	H123—C13A—H121	102 (4)
H3B3—C3B—H3B2	109 (3)	C11A—C13A—H122	105 (2)
C2B—C3B—H3B1	108 (3)	H123—C13A—H122	115 (5)
H3B3—C3B—H3B1	109 (4)	H121—C13A—H122	114 (3)
H3B2—C3B—H3B1	109 (3)	C11A—C12A—H133	110 (3)
C11B—C13B—H136	98 (3)	C11A—C12A—H132	104 (3)
C11B—C13B—H134	109 (3)	H133—C12A—H132	111 (4)
H136—C13B—H134	106 (4)	C11A—C12A—H131	106 (2)
C11B—C13B—H135	114 (3)	H133—C12A—H131	113 (4)
H136—C13B—H135	117 (4)	H132—C12A—H131	112 (4)

C5B—C4B—C9B—C8B	−1.1 (4)	O2A—C1A—C2A—C4A	95.9 (4)
C2B—C4B—C9B—C8B	179.3 (3)	O1A—C1A—C2A—C4A	−81.7 (4)
C8B—C7B—C6B—C5B	−1.4 (4)	O2A—C1A—C2A—C3A	−29.6 (5)
C10B—C7B—C6B—C5B	177.7 (3)	O1A—C1A—C2A—C3A	152.8 (3)
C4B—C9B—C8B—C7B	−0.5 (4)	C1A—C2A—C4A—C9A	−85.5 (4)
C6B—C7B—C8B—C9B	1.7 (4)	C3A—C2A—C4A—C9A	38.7 (4)
C10B—C7B—C8B—C9B	−177.3 (3)	C1A—C2A—C4A—C5A	91.4 (4)
C9B—C4B—C2B—C1B	84.3 (3)	C3A—C2A—C4A—C5A	−144.4 (4)
C5B—C4B—C2B—C1B	−95.3 (3)	C9A—C4A—C5A—C6A	−1.2 (5)
C9B—C4B—C2B—C3B	−151.3 (3)	C2A—C4A—C5A—C6A	−178.3 (3)
C5B—C4B—C2B—C3B	29.1 (4)	C4A—C5A—C6A—C7A	0.5 (6)
C7B—C6B—C5B—C4B	−0.2 (5)	C5A—C6A—C7A—C8A	0.4 (5)
C9B—C4B—C5B—C6B	1.4 (4)	C5A—C6A—C7A—C10A	−177.0 (3)
C2B—C4B—C5B—C6B	−178.9 (3)	C6A—C7A—C8A—C9A	−0.5 (5)
C8B—C7B—C10B—C11B	101.8 (3)	C10A—C7A—C8A—C9A	176.8 (3)
C6B—C7B—C10B—C11B	−77.2 (4)	C7A—C8A—C9A—C4A	−0.2 (5)
C7B—C10B—C11B—C12B	−68.0 (5)	C5A—C4A—C9A—C8A	1.1 (5)
C7B—C10B—C11B—C13B	168.3 (4)	C2A—C4A—C9A—C8A	178.1 (3)
C4B—C2B—C1B—O2B	−94.6 (3)	C8A—C7A—C10A—C11A	−93.2 (5)
C3B—C2B—C1B—O2B	139.2 (3)	C6A—C7A—C10A—C11A	84.0 (5)
C4B—C2B—C1B—O1B	83.5 (3)	C7A—C10A—C11A—C13A	67.9 (5)
C3B—C2B—C1B—O1B	−42.7 (4)	C7A—C10A—C11A—C12A	−168.7 (4)