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

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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.

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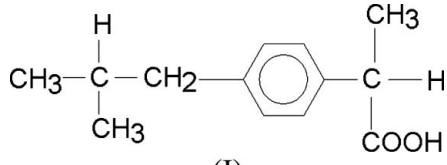
In the paper by Hansen, Perlovich & Bauer-Brandl [*Acta Cryst.* (2003), E**59**, o1357–o1358], the coordinates of the *R* enantiomer of the title compound, $C_{13}H_{18}O_2$, were incorrectly given instead of those of the *S* enantiomer. The correct coordinates of the *S* enantiomer are given here.

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.

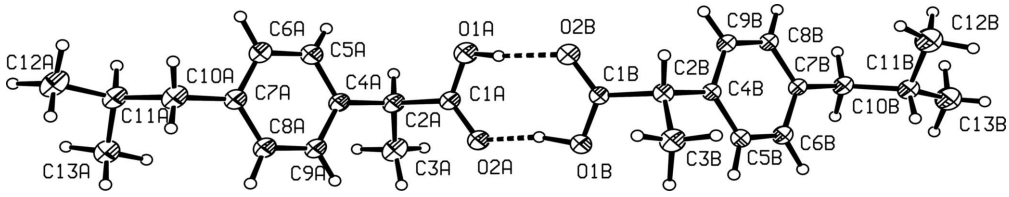


Figure 1
The structure of the two independent molecules of (I). Displacement ellipsoids are shown at the 30% probability level. Hydrogen bonds are shown as dashed lines.

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