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(–)-(1*R*,2*S*,2′*R*,5*R*)-2-(1-Hydroxy-prop-2-yl)-5-methylcyclohexanol. Corrigendum

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The crystal structure of the title compound, $C_{10}H_{20}O_2$, was published [Körner *et al.* (2000). *Acta Cryst.* C**56**, 74–75] with an erroneous position for an hydroxy H atom. This has now been corrected and leads to a more sensible hydrogen-bonding scheme.

Comment

In the original publication of the crystal structure of the title compound (Körner *et al.*, 2000), an erroneous position for a hydroxyl H atom was reported, which was detected with *PLATON* (Spek, 2000). A new refinement with merged Friedel data (the original analysis was carried out with an unmerged data set), the correct location for the hydroxy H1 atom and the additional introduction of an extinction correction, led to significant improvement in the structural results. Details of the correct hydrogen-bonding scheme are given in Table 1. Molecules are joined in a hydrogen-bonded chain running in the *b*-axis direction.

Experimental

Crystal data

$C_{10}H_{20}O_2$
M_r = 172.26
Monoclinic, $P2_1$
a = 8.5710 (7) Å
b = 6.4665 (3) Å
c = 9.8502 (8) Å
β = 106.783 (3)°
V = 522.69 (6) Å^3
Z = 2
D_x = 1.095 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6694 reflections
θ = 3.73–25.76°
μ = 0.074 mm^{-1}
T = 291 (1) K
Needle, colourless
0.30 × 0.08 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Method: 360 frames *via* ω rotation ($\Delta\omega$ = 1°) and two times 60 s per frame
6694 measured reflections
1065 independent reflections
761 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.76°
$h = -10 \rightarrow 10$
$k = -7 \rightarrow 7$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.081
S = 1.012
1065 reflections
114 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.0006P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.08 e Å^{-3}
$\Delta\rho_{min}$ = −0.10 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.060 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1^{i}	0.82	1.84	2.660 (2)	174
O1′—H1′···O1^{ii}	0.82	1.90	2.712 (2)	173

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

H atoms were treated as riding with distances and displacement parameters set as follows: O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O), Csp—H = 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C), Csp^2—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C), and Csp^3—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C).

Data collection: *KappaCCD Software* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1996); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1383). Services for accessing these data are described at the back of the journal.

References

Körner, F., Schürmann, M., Preut, H. & Kreiser, W. (2000). *Acta Cryst.* C**56**, 74–75.
Nonius (1998). *KappaCCD Software*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1996). *Methods Enzymol.* **276**, 307–326.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2000). *PLATON*. Utrecht University, The Netherlands.

