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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.

supporting information

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Computing details

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(-)-(1*R*,2S,2′*R*,5*R*)-2-(1-Hydroxyprop-2-yl)-5-methylcyclohexanol

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Monoclinic, $P2_1$
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$c = 9.8502\ (8)$ Å
$\beta = 106.783\ (3)°$
$V = 522.69\ (6)$ Å^3
$Z = 2$
$F(000) = 192$
$D_x = 1.095$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 6694 reflections
$\theta = 3.7–25.8°$
$\mu = 0.07$ mm^{-1}
$T = 291$ K
Needle, colourless
0.30 × 0.08 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 19 vertical, 18 horizontal pixels mm^{-1}
360 frames via ω–rotation ($\Delta\omega = 1°$) and two times 60 s per frame scans
6694 measured reflections
1065 independent reflections
761 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 25.8°$, $\theta_{min} = 3.7°$
$h = -10\rightarrow10$
$k = -7\rightarrow7$
$l = -11\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.081$
$S = 1.01$
1065 reflections
114 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
Calculated $w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.0006P]$ 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: *SHELXL97*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.060 (13)

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}
O1	0.40833 (18)	0.3316 (2)	0.35093 (19)	0.0553 (5)
H1	0.4230	0.4567	0.3605	0.083*
O1′	0.4694 (2)	−0.2645 (2)	0.37048 (18)	0.0678 (6)
H1′	0.5129	−0.2297	0.4528	0.102*
C1	0.2434 (2)	0.2922 (3)	0.2694 (2)	0.0450 (6)
H1A	0.2238	0.3614	0.1775	0.054*
C1′	0.4989 (3)	−0.1110 (4)	0.2770 (3)	0.0592 (6)
H1′1	0.5702	−0.1672	0.2256	0.071*
H1′2	0.5534	0.0065	0.3318	0.071*
C2	0.2225 (3)	0.0607 (3)	0.2438 (2)	0.0446 (6)
H2	0.2411	−0.0048	0.3368	0.053*
C2′	0.3418 (3)	−0.0403 (3)	0.1730 (2)	0.0502 (6)
H2′	0.2877	−0.1650	0.1254	0.060*
C3	0.0450 (3)	0.0174 (4)	0.1604 (2)	0.0609 (7)
H3A	0.0236	0.0765	0.0663	0.073*
H3B	0.0292	−0.1309	0.1499	0.073*
C3′	0.3791 (3)	0.0932 (4)	0.0584 (3)	0.0681 (8)
H3′1	0.4409	0.2121	0.1014	0.102*
H3′2	0.2789	0.1373	−0.0079	0.102*
H3′3	0.4410	0.0140	0.0096	0.102*
C4	−0.0768 (3)	0.1050 (4)	0.2310 (3)	0.0659 (8)
H4A	−0.1864	0.0805	0.1704	0.079*
H4B	−0.0651	0.0334	0.3199	0.079*
C5	−0.0529 (3)	0.3352 (4)	0.2594 (3)	0.0601 (7)
H5	−0.0746	0.4055	0.1677	0.072*
C5A	−0.1712 (3)	0.4215 (6)	0.3354 (3)	0.0899 (10)
H5A1	−0.2812	0.3947	0.2795	0.135*
H5A2	−0.1551	0.5680	0.3481	0.135*
H5A3	−0.1516	0.3561	0.4263	0.135*
C6	0.1243 (3)	0.3769 (4)	0.3423 (2)	0.0553 (6)
H6A	0.1406	0.5249	0.3548	0.066*
H6B	0.1465	0.3149	0.4356	0.066*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0504 (10)	0.0389 (8)	0.0707 (11)	−0.0058 (7)	0.0085 (8)	−0.0043 (7)
O1′	0.0800 (13)	0.0374 (9)	0.0742 (12)	−0.0061 (8)	0.0038 (10)	0.0021 (8)
C1	0.0415 (13)	0.0419 (13)	0.0489 (13)	−0.0007 (10)	0.0087 (11)	0.0020 (10)
C1′	0.0589 (16)	0.0423 (13)	0.0765 (16)	−0.0006 (11)	0.0199 (13)	−0.0046 (12)
C2	0.0465 (14)	0.0391 (13)	0.0463 (12)	−0.0045 (10)	0.0105 (11)	0.0007 (10)
C2′	0.0532 (15)	0.0404 (13)	0.0562 (14)	−0.0031 (10)	0.0145 (12)	−0.0073 (10)
C3	0.0564 (17)	0.0560 (14)	0.0681 (16)	−0.0105 (12)	0.0146 (14)	−0.0116 (13)
C3′	0.0762 (18)	0.0692 (18)	0.0643 (16)	0.0017 (13)	0.0288 (14)	−0.0007 (13)
C4	0.0457 (15)	0.0751 (18)	0.0748 (17)	−0.0080 (12)	0.0142 (13)	−0.0043 (14)
C5	0.0526 (15)	0.0684 (17)	0.0587 (15)	0.0093 (13)	0.0153 (12)	0.0021 (13)
C5A	0.063 (2)	0.112 (3)	0.098 (2)	0.0151 (17)	0.0303 (17)	−0.014 (2)
C6	0.0590 (15)	0.0466 (14)	0.0590 (14)	0.0036 (11)	0.0150 (12)	−0.0039 (11)

Geometric parameters (Å, º)

O1—C1	1.433 (3)	C3—H3A	0.9700
O1—H1	0.8200	C3—H3B	0.9700
O1′—C1′	1.425 (3)	C3′—H3′1	0.9600
O1′—H1′	0.8200	C3′—H3′2	0.9600
C1—C6	1.510 (3)	C3′—H3′3	0.9600
C1—C2	1.520 (3)	C4—C5	1.517 (4)
C1—H1A	0.9800	C4—H4A	0.9700
C1′—C2′	1.508 (3)	C4—H4B	0.9700
C1′—H1′1	0.9700	C5—C6	1.527 (3)
C1′—H1′2	0.9700	C5—C5A	1.529 (3)
C2—C3	1.532 (3)	C5—H5	0.9800
C2—C2′	1.539 (3)	C5A—H5A1	0.9600
C2—H2	0.9800	C5A—H5A2	0.9600
C2′—C3′	1.527 (3)	C5A—H5A3	0.9600
C2′—H2′	0.9800	C6—H6A	0.9700
C3—C4	1.521 (3)	C6—H6B	0.9700
C1—O1—H1	109.5	H3A—C3—H3B	107.8
C1′—O1′—H1′	109.5	C2′—C3′—H3′1	109.5
O1—C1—C6	111.23 (18)	C2′—C3′—H3′2	109.5
O1—C1—C2	108.52 (16)	H3′1—C3′—H3′2	109.5
C6—C1—C2	111.91 (19)	C2′—C3′—H3′3	109.5
O1—C1—H1A	108.4	H3′1—C3′—H3′3	109.5
C6—C1—H1A	108.4	H3′2—C3′—H3′3	109.5
C2—C1—H1A	108.4	C5—C4—C3	112.1 (2)
O1′—C1′—C2′	111.09 (18)	C5—C4—H4A	109.2
O1′—C1′—H1′1	109.4	C3—C4—H4A	109.2
C2′—C1′—H1′1	109.4	C5—C4—H4B	109.2
O1′—C1′—H1′2	109.4	C3—C4—H4B	109.2
C2′—C1′—H1′2	109.4	H4A—C4—H4B	107.9

H1′1—C1′—H1′2	108.0	C4—C5—C6	109.4 (2)
C1—C2—C3	108.66 (19)	C4—C5—C5A	112.0 (3)
C1—C2—C2′	115.59 (19)	C6—C5—C5A	111.8 (2)
C3—C2—C2′	111.53 (17)	C4—C5—H5	107.8
C1—C2—H2	106.9	C6—C5—H5	107.8
C3—C2—H2	106.9	C5A—C5—H5	107.8
C2′—C2—H2	106.9	C5—C5A—H5A1	109.5
C1′—C2′—C3′	109.70 (19)	C5—C5A—H5A2	109.5
C1′—C2′—C2	113.63 (18)	H5A1—C5A—H5A2	109.5
C3′—C2′—C2	113.79 (19)	C5—C5A—H5A3	109.5
C1′—C2′—H2′	106.4	H5A1—C5A—H5A3	109.5
C3′—C2′—H2′	106.4	H5A2—C5A—H5A3	109.5
C2—C2′—H2′	106.4	C1—C6—C5	112.73 (18)
C4—C3—C2	113.2 (2)	C1—C6—H6A	109.0
C4—C3—H3A	108.9	C5—C6—H6A	109.0
C2—C3—H3A	108.9	C1—C6—H6B	109.0
C4—C3—H3B	108.9	C5—C6—H6B	109.0
C2—C3—H3B	108.9	H6A—C6—H6B	107.8
O1—C1—C2—C3	178.33 (17)	C1—C2—C3—C4	−54.5 (3)
C6—C1—C2—C3	55.2 (2)	C2′—C2—C3—C4	177.0 (2)
O1—C1—C2—C2′	−55.4 (2)	C2—C3—C4—C5	55.2 (3)
C6—C1—C2—C2′	−178.56 (18)	C3—C4—C5—C6	−53.2 (3)
O1′—C1′—C2′—C3′	−169.72 (18)	C3—C4—C5—C5A	−177.8 (2)
O1′—C1′—C2′—C2	61.7 (2)	O1—C1—C6—C5	−179.2 (2)
C1—C2—C2′—C1′	88.2 (2)	C2—C1—C6—C5	−57.6 (2)
C3—C2—C2′—C1′	−147.1 (2)	C4—C5—C6—C1	55.1 (3)
C1—C2—C2′—C3′	−38.3 (3)	C5A—C5—C6—C1	179.8 (2)
C3—C2—C2′—C3′	86.4 (2)		

Hydrogen-bond geometry (Å, º)

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*, *y*+1, *z*; (ii) −*x*+1, *y*−1/2, −*z*+1.