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(*S*,*S*)-2,2′-(1,2-Ethanediyldiimino)dibutan-1-ol. Corrigendum

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In the paper by Bai, Zhang, Zhang, Zeng & Li [*Acta Cryst.* (2006), E**62**, o2173–o2174], the data relate to the *R*,*R* rather than the *S*,*S* enantiomer. The revised ellipsoid plot, packing diagram and selected geometrical data are given here.

Experimental

Data collection

R_{int} = 0.029

Refinement

$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.0456P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.419 (3)		
C2—N1—C5	115.4 (2)	N1—C5—C6	109.7 (2)
N1—C2—C1	108.3 (2)		
O1—C1—C2—N1	−61.4 (3)	N1—C5—C6—N2	173.0 (2)
N1—C2—C3—C4	−162.1 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2^{i}	0.93 (5)	1.95 (5)	2.877 (3)	174 (3)
O2—H2*B*···N1^{ii}	0.96 (4)	1.82 (4)	2.767 (3)	174 (3)
N1—H1*C*···O2^{iii}	0.85 (3)	2.23 (3)	3.014 (3)	153 (3)

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

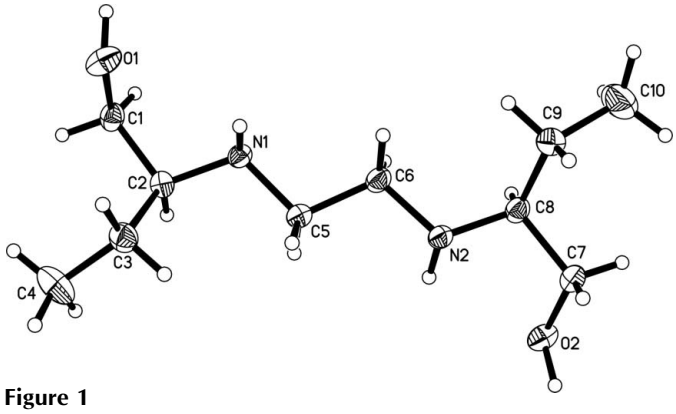

Figure 1
The molecular structure of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids.

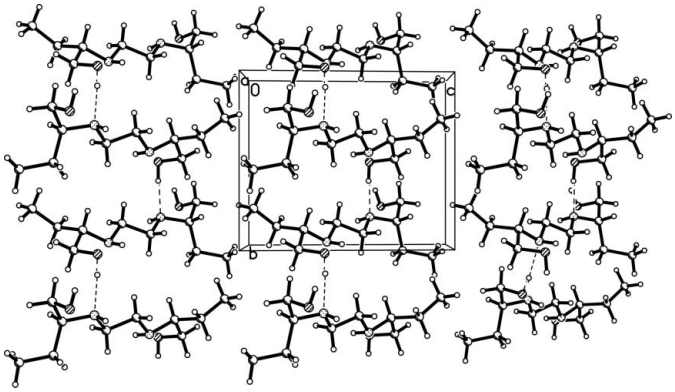

Figure 2
Packing diagram for (I), with hydrogen bonds shown as dashed lines.

supporting information

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(*S*,*S*)-2,2′-(1,2-Ethanediyldiimino)dibutan-1-ol. Corrigendum

Guo-Yi Bai, Chen-Fang Zhang, Yue-Cheng Zhang, Tao Zeng and Jiang-Sheng Li

(*S*,*S*)-2,2′-(1,2-Ethanediyldiimino)bis-1-butanol

Crystal data

$C_{10}H_{24}N_2O_2$
$M_r = 204.31$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 7.157$ (3) Å
$b = 8.440$ (4) Å
$c = 10.193$ (5) Å
$\beta = 95.631$ (8)°
$V = 612.7$ (5) Å^3
$Z = 2$
$F(000) = 228$
$D_x = 1.107$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1264 reflections
$\theta = 2.9$–25.3°
$\mu = 0.08$ mm^{-1}
$T = 294$ K
Block, colourless
0.22 × 0.20 × 0.10 mm

Data collection

Bruker SMART-1000 CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan SADABS (Sheldrick, 1996)
$T_{min} = 0.979$, $T_{max} = 0.992$
3317 measured reflections
1318 independent reflections
1049 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 26.3°$, $\theta_{min} = 2.0°$
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 6$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.103$
$S = 1.07$
1318 reflections
141 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.0456P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Absolute structure: Friedel pairs merged

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	0.1972 (3)	0.7636 (3)	0.6659 (2)	0.0496 (6)
H1	0.145 (5)	0.667 (6)	0.639 (3)	0.074*
O2	1.3357 (3)	1.0029 (3)	0.39638 (19)	0.0421 (5)
H2B	1.376 (4)	1.111 (5)	0.400 (3)	0.063*
N1	0.5708 (3)	0.8209 (3)	0.6068 (2)	0.0303 (5)
H1C	0.481 (4)	0.845 (4)	0.549 (3)	0.036*
N2	0.9494 (3)	0.9540 (3)	0.4033 (2)	0.0316 (5)
H2A	1.036 (4)	0.964 (4)	0.473 (3)	0.038*
C1	0.3535 (3)	0.7352 (3)	0.7597 (3)	0.0373 (7)
H1A	0.3962	0.6269	0.7514	0.045*
H1B	0.3162	0.7489	0.8480	0.045*
C2	0.5125 (3)	0.8485 (3)	0.7386 (2)	0.0319 (6)
H2	0.6188	0.8190	0.8019	0.038*
C3	0.4630 (4)	1.0212 (4)	0.7683 (3)	0.0422 (7)
H3A	0.5529	1.0907	0.7321	0.051*
H3B	0.3398	1.0452	0.7244	0.051*
C4	0.4627 (6)	1.0550 (5)	0.9136 (3)	0.0697 (11)
H4A	0.5803	1.0225	0.9590	0.105*
H4B	0.3623	0.9976	0.9477	0.105*
H4C	0.4453	1.1665	0.9265	0.105*
C5	0.7343 (3)	0.9135 (3)	0.5739 (3)	0.0356 (6)
H5A	0.8345	0.9052	0.6448	0.043*
H5B	0.6998	1.0243	0.5634	0.043*
C6	0.8011 (4)	0.8520 (3)	0.4479 (3)	0.0348 (6)
H6A	0.8492	0.7452	0.4619	0.042*
H6B	0.6962	0.8477	0.3801	0.042*
C7	1.2165 (4)	0.9866 (4)	0.2782 (2)	0.0394 (7)
H7A	1.2866	0.9407	0.2109	0.047*
H7B	1.1730	1.0904	0.2480	0.047*
C8	1.0489 (4)	0.8826 (3)	0.2974 (2)	0.0342 (6)
H8	1.0935	0.7770	0.3254	0.041*
C9	0.9224 (4)	0.8677 (4)	0.1694 (3)	0.0482 (8)
H9A	0.8030	0.8236	0.1888	0.058*
H9B	0.8984	0.9729	0.1333	0.058*
C10	1.0003 (5)	0.7663 (6)	0.0660 (3)	0.0861 (15)
H10A	1.0407	0.6664	0.1040	0.129*
H10B	1.1052	0.8191	0.0334	0.129*
H10C	0.9048	0.7486	−0.0054	0.129*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0365 (11)	0.0386 (12)	0.0726 (14)	−0.0050 (10)	−0.0011 (10)	0.0063 (11)
O2	0.0349 (10)	0.0396 (12)	0.0505 (11)	−0.0049 (9)	−0.0030 (8)	0.0096 (10)
N1	0.0256 (10)	0.0333 (13)	0.0319 (11)	−0.0017 (10)	0.0018 (9)	0.0012 (10)
N2	0.0311 (11)	0.0287 (12)	0.0356 (12)	−0.0047 (10)	0.0056 (9)	−0.0016 (10)
C1	0.0386 (15)	0.0332 (16)	0.0416 (15)	0.0007 (13)	0.0120 (12)	0.0038 (12)
C2	0.0333 (13)	0.0322 (15)	0.0305 (13)	0.0050 (12)	0.0040 (11)	0.0025 (11)
C3	0.0461 (15)	0.0341 (16)	0.0472 (16)	0.0037 (14)	0.0087 (13)	−0.0033 (14)
C4	0.095 (3)	0.058 (2)	0.056 (2)	0.019 (2)	0.0038 (19)	−0.0184 (17)
C5	0.0331 (13)	0.0349 (15)	0.0393 (14)	−0.0063 (13)	0.0062 (11)	−0.0039 (12)
C6	0.0341 (13)	0.0305 (14)	0.0407 (14)	−0.0052 (12)	0.0081 (12)	0.0011 (12)
C7	0.0369 (14)	0.0418 (17)	0.0403 (14)	−0.0066 (13)	0.0080 (11)	0.0022 (13)
C8	0.0348 (14)	0.0293 (15)	0.0395 (14)	−0.0025 (12)	0.0091 (12)	0.0013 (12)
C9	0.0426 (16)	0.058 (2)	0.0442 (16)	−0.0096 (16)	0.0061 (13)	−0.0104 (15)
C10	0.075 (2)	0.116 (4)	0.070 (2)	−0.012 (3)	0.019 (2)	−0.045 (3)

Geometric parameters (Å, º)

O1—C1	1.419 (3)	C4—H4B	0.9600
O1—H1	0.93 (5)	C4—H4C	0.9600
O2—C7	1.412 (3)	C5—C6	1.506 (4)
O2—H2B	0.96 (4)	C5—H5A	0.9700
N1—C2	1.464 (3)	C5—H5B	0.9700
N1—C5	1.473 (3)	C6—H6A	0.9700
N1—H1C	0.85 (3)	C6—H6B	0.9700
N2—C6	1.473 (3)	C7—C8	1.515 (4)
N2—C8	1.478 (3)	C7—H7A	0.9700
N2—H2A	0.90 (3)	C7—H7B	0.9700
C1—C2	1.518 (4)	C8—C9	1.519 (4)
C1—H1A	0.9700	C8—H8	0.9800
C1—H1B	0.9700	C9—C10	1.507 (4)
C2—C3	1.536 (4)	C9—H9A	0.9700
C2—H2	0.9800	C9—H9B	0.9700
C3—C4	1.508 (4)	C10—H10A	0.9600
C3—H3A	0.9700	C10—H10B	0.9600
C3—H3B	0.9700	C10—H10C	0.9600
C4—H4A	0.9600		
C1—O1—H1	109 (2)	C6—C5—H5A	109.7
C7—O2—H2B	106.1 (19)	N1—C5—H5B	109.7
C2—N1—C5	115.4 (2)	C6—C5—H5B	109.7
C2—N1—H1C	109.3 (17)	H5A—C5—H5B	108.2
C5—N1—H1C	106.3 (19)	N2—C6—C5	111.1 (2)
C6—N2—C8	113.6 (2)	N2—C6—H6A	109.4
C6—N2—H2A	106.0 (17)	C5—C6—H6A	109.4
C8—N2—H2A	105.8 (16)	N2—C6—H6B	109.4

O1—C1—C2	110.6 (2)	C5—C6—H6B	109.4
O1—C1—H1A	109.5	H6A—C6—H6B	108.0
C2—C1—H1A	109.5	O2—C7—C8	111.5 (2)
O1—C1—H1B	109.5	O2—C7—H7A	109.3
C2—C1—H1B	109.5	C8—C7—H7A	109.3
H1A—C1—H1B	108.1	O2—C7—H7B	109.3
N1—C2—C1	108.3 (2)	C8—C7—H7B	109.3
N1—C2—C3	115.1 (2)	H7A—C7—H7B	108.0
C1—C2—C3	112.3 (2)	N2—C8—C7	107.6 (2)
N1—C2—H2	106.9	N2—C8—C9	111.8 (2)
C1—C2—H2	106.9	C7—C8—C9	110.5 (2)
C3—C2—H2	106.9	N2—C8—H8	109.0
C4—C3—C2	113.3 (3)	C7—C8—H8	109.0
C4—C3—H3A	108.9	C9—C8—H8	109.0
C2—C3—H3A	108.9	C10—C9—C8	114.7 (3)
C4—C3—H3B	108.9	C10—C9—H9A	108.6
C2—C3—H3B	108.9	C8—C9—H9A	108.6
H3A—C3—H3B	107.7	C10—C9—H9B	108.6
C3—C4—H4A	109.5	C8—C9—H9B	108.6
C3—C4—H4B	109.5	H9A—C9—H9B	107.6
H4A—C4—H4B	109.5	C9—C10—H10A	109.5
C3—C4—H4C	109.5	C9—C10—H10B	109.5
H4A—C4—H4C	109.5	H10A—C10—H10B	109.5
H4B—C4—H4C	109.5	C9—C10—H10C	109.5
N1—C5—C6	109.7 (2)	H10A—C10—H10C	109.5
N1—C5—H5A	109.7	H10B—C10—H10C	109.5

C5—N1—C2—C1	−175.7 (2)	N1—C5—C6—N2	173.0 (2)
C5—N1—C2—C3	57.8 (3)	C6—N2—C8—C7	−170.5 (2)
O1—C1—C2—N1	−61.4 (3)	C6—N2—C8—C9	68.0 (3)
O1—C1—C2—C3	66.7 (3)	O2—C7—C8—N2	57.3 (3)
N1—C2—C3—C4	−162.1 (3)	O2—C7—C8—C9	179.7 (2)
C1—C2—C3—C4	73.4 (3)	N2—C8—C9—C10	−167.9 (3)
C2—N1—C5—C6	169.3 (2)	C7—C8—C9—C10	72.3 (4)
C8—N2—C6—C5	167.6 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2^{i}	0.93 (5)	1.95 (5)	2.877 (3)	174 (3)
O2—H2*B*···N1^{ii}	0.96 (4)	1.81 (4)	2.767 (3)	174 (3)
N1—H1*C*···O2^{iii}	0.85 (3)	2.23 (3)	3.014 (3)	153 (3)

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1; (ii) −*x*+2, *y*+1/2, −*z*+1; (iii) *x*−1, *y*, *z*.