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(*RS*)-2,3-Dibromosuccinic acid. Erratum

Margareta Eriksson,[a] Andreas Fischer,[a]* Johan Lind[b] and Åsa Zazzi[a]

[a]Inorganic Chemistry, School of Chemical Science and Engineering, Royal Institute of Technology, 100 44 Stockholm, Sweden, and [b]Nuclear Chemistry, School of Chemical Science and Engineering, Royal Institute of Technology, 100 44 Stockholm, Sweden

Correspondence e-mail: andif@inorg.kth.se

In the paper by Eriksson, Fischer, Lind & Zazzi [*Acta Cryst.* (2006), E**62**, o200–o201], the correct name of the title compound is '(2*R*,3*S*)-2,3-Dibromosuccinic acid'.

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(2*R*,3*S*)-2,3-Dibromosuccinic acid

Margareta Eriksson,[a] Andreas Fischer,[a]* Johan Lind[b] and Åsa Zazzi[a]

[a]Inorganic Chemistry, School of Chemical Science and Engineering, Royal Institute of Technology, 100 44 Stockholm, Sweden, and [b]Nuclear Chemistry, School of Chemical Science and Engineering, Royal Institute of Technology, 100 44 Stockholm, Sweden

Correspondence e-mail: andif@inorg.kth.se

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.013 Å
R factor = 0.045
wR factor = 0.102
Data-to-parameter ratio = 18.1

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

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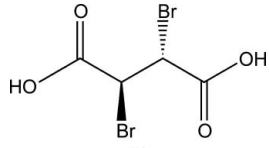
Crystals of the title compound, $C_4H_4Br_2O_4$, were grown from an aqueous solution. The structure features centrosymmetric molecules, each of which forms hydrogen bonds with two adjacent acid molecules, yielding long chains.

Comment

Some time ago, the structure of racemic 2,3-dibromosuccinic acid, which had been obtained by an electrophilic reaction between maleic acid and bromine, was determined (Bolte & Degen, 2000). The structure features a complex pattern of hydrogen bonds between carboxy groups of adjacent acid molecules. Inspired by the fact that the melting points of the racemic and the meso compounds are extremely different (racemate: 444 K; meso compound: 528 K), we expected very different hydrogen-bonding patterns in the two phases and decided therefore to determine the structure of the meso compound. From a reaction between bromine and fumaric acid, we obtained single crystals of the meso compound, (I), whose structure is described here. The molecule lies about an inversion centre located at the mid-point of the C2—C2^{i} bond [symmetry code: (i) $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$]. The geometry of the molecule is essentially the same as in the structure of pyridone–(*RS*)-2,3-dibromosuccinic acid (1:1) (Aakeröy *et al.*, 2000). In the crystal structure, the carboxy groups link pairs of molecules, forming an inversion-related closed hydrogen-bonding loop and infinite chains along the *a* axis (Fig. 2).



(I)

Experimental

An aqueous solution (2.5 ml) containing 0.69 mol l^{-1} of fumaric acid, 2.1 mol l^{-1} of KBr and 1.9 mol l^{-1} of Br_2 was placed in a boiling water bath. To avoid precipitation of KBr, the volume of the solution was kept constant by addition of deionized water. After 10 min, crystals of (I) were vacuum-filtered and placed in a heated cabinet at 373 K for 1 h.

Crystal data

$C_4H_4Br_2O_4$
M_r = 275.89
Monoclinic, *C*2/*c*
a = 14.244 (1) Å
b = 5.1664 (6) Å
c = 11.3736 (8) Å
β = 117.684 (9)°
V = 741.17 (13) Å^3
Z = 4
D_x = 2.477 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 37 reflections
θ = 4.3–21.0°
μ = 10.91 mm^{-1}
T = 298 K
Block, colourless
0.33 × 0.30 × 0.27 mm

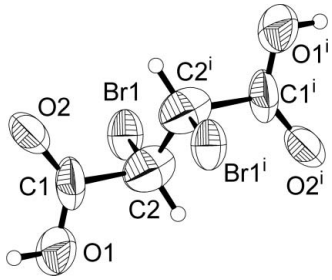


Figure 1
The (*R*,*S*)-2,3-dibromosuccinic acid molecule. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (i) $\frac{1}{2}-x,\frac{1}{2}-y,1-z$].

Data collection

Bruker–Nonius KappaCCD diffractometer	849 independent reflections
φ scans	679 reflections with $I > 2\sigma(I)$
Absorption correction: numerical *HABITUS* (Herrendorf & Bärnighausen, 1997)	$R_{int} = 0.039$
$T_{min} = 0.091$, $T_{max} = 0.137$	$\theta_{max} = 27.5°$
5265 measured reflections	$h = -15 \rightarrow 18$
	$k = -6 \rightarrow 6$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0299P)^2 + 8.0961P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.102$	$\Delta\rho_{max} = 1.14$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.73$ e Å^{-3}
849 reflections	
47 parameters	
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

Br1—C2	1.969 (8)	C1—C2	1.605 (11)
O1—C1	1.229 (10)	C2—C2^{i}	1.403 (16)
O2—C1	1.244 (9)		

Symmetry code: (i) $-x+\frac{1}{2},-y+\frac{1}{2},-z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{ii}	0.82	1.83	2.650 (7)	175

Symmetry code: (ii) $-x,-y,-z+1$.

The H atoms were located in a difference Fourier map and were refined using a riding model, with C—H = 0.96 Å and U_{iso}(H) = $1.2U_{eq}$(C), and with O—H = 0.82 Å and U_{iso}(H) = $1.5U_{eq}$(O). The highest peak is located 0.97 Å from atom C2.

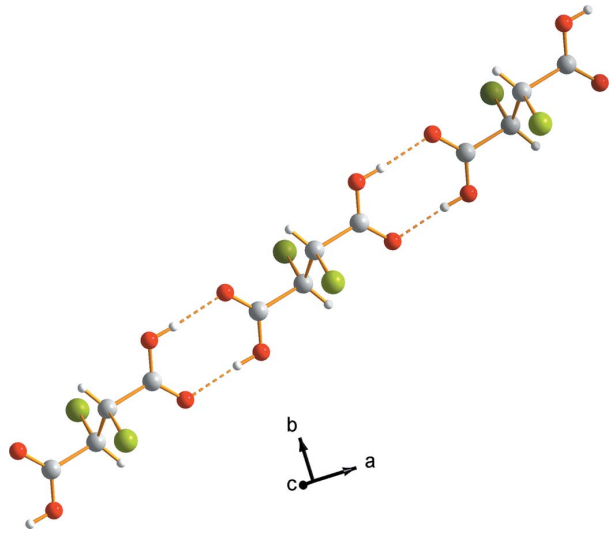


Figure 2
The chains formed by hydrogen bonds in (I). Hydrogen bonds are indicated by dashed lines.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2003); data reduction: *EVALCCD* (Duisenberg, 1992); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *MAXUS* (Mackay *et al.*, 1999).

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