

Tetrakis[(*R*)-lactamide- κ^2 O,*O'*]-strontium(II) dibromide

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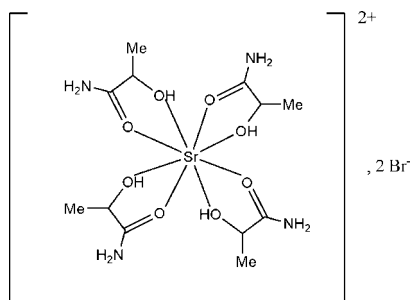
Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.045; wR factor = 0.111; data-to-parameter ratio = 26.2.

The title compound, $[\text{Sr}(\text{C}_3\text{H}_7\text{NO}_2)_4]\text{Br}_2$, contains one monomeric octacoordinated strontium complex cation and two Br^- anions. The Sr atom lies on a twofold axis. Coordination occurs *via* the amide [similar Sr—O: average 2.539 (4) Å] and hydroxy O atoms [Sr—O = 2.535 (4)–2.703 (3) Å], and the geometry may be described as a distorted square-antiprismatic arrangement with the Sr atom located 1.481 (2) Å away from the least-squares planes of the two symmetry-related square bases. In the crystal structure, the cations and anions are linked by N—H...Br and O—H...Br hydrogen bonds, generating a three-dimensional network.

Related literature

The crystal structure of tetra[(*R*)-lactamide- κ^2 O,*O'*]-strontium(II) dibromide was compared with bis[(*R*)-lactamido- κ^2 O,*O'*]boron(III) bromide (Bekaert *et al.*, 2007) and tris[(*R*)-lactamido- κ^2 O,*O'*]zinc(II) tetrabromozincate(II) (Bekaert *et al.*, 2005).

For related literature, see: Finlay *et al.* (2005); Makhijani (2003); Reginster *et al.* (2007); Stahl *et al.* (2006).



Experimental

Crystal data

$[\text{Sr}(\text{C}_3\text{H}_7\text{NO}_2)_4]\text{Br}_2$
 $M_r = 603.82$
 Orthorhombic, $P2_12_12$
 $a = 10.385$ (2) Å
 $b = 17.919$ (2) Å
 $c = 6.308$ (1) Å

$V = 1173.8$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 5.74$ mm⁻¹
 $T = 293$ (2) K
 $0.25 \times 0.16 \times 0.12$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 Absorption correction: multi-scan (Blessing, 1995)
 $T_{\min} = 0.27$, $T_{\max} = 0.50$
 7106 measured reflections

3407 independent reflections
 2379 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.067$
 3 standard reflections
 frequency: 60 min
 intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.111$
 $S = 0.99$
 3407 reflections
 130 parameters
 2 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.68$ e Å⁻³
 $\Delta\rho_{\min} = -1.77$ e Å⁻³
 Absolute structure: Flack (1983), 1433 Friedel pairs
 Flack parameter: -0.017 (15)

Table 1

Selected bond lengths (Å).

Sr1—O1	2.533 (3)	Sr1—O6	2.544 (4)
Sr1—O2	2.535 (4)	Sr1—O7	2.703 (3)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O7—H7A...Br2	0.82 (4)	2.43 (3)	3.203 (4)	158 (6)
N1—H1A...Br2 ⁱ	0.86	2.72	3.572 (5)	171
N1—H1B...Br2 ⁱⁱ	0.86	2.73	3.568 (5)	167
O2—H2A...O6 ⁱⁱⁱ	0.82 (4)	1.95 (4)	2.759 (5)	169 (6)
N6—H6A...O7 ^{iv}	0.86	2.24	3.071 (6)	161
N6—H6B...Br2 ^v	0.86	2.59	3.424 (5)	164

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *WinGX* (Version 1.63.02; Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2119).

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supplementary materials

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Tetrakis[(*R*)-lactamide- κ^2 O,*O'*]strontium(II) dibromide

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Comment

Strontium provides some of the most important radioactive isotopes in the environment; *e.g.*, ^{90}Sr (Finlay *et al.*, 2005), a by-product of the fission of uranium and plutonium in nuclear reaction or nuclear weapons, of which large amounts were produced during the Tchernobyl nuclear power plant disaster in 1986. It was later found in milk and vegetables. It is chemically similar to calcium and tends to deposit in bones and teeth. The half-life of ^{90}Sr is 29.1 years emitting beta particules. Another isotope, ^{89}Sr , is the active ingredient in Metaston^{pe.g}, a radiopharmaceutical used for bone pain secondary to metastatic prostate cancer (Makhijani, 2003). Cold strontium ranelate (Prodelos^{pe.g}) is the first antiosteoporotic treatment to simultaneously increase bone formation and decrease bone resorption (Reginster *et al.*, 2007). In order to find new ligands of strontium as osteoporosous drugs, a new complex of strontium dibromide and *R*-lactamide has been studied. Compound (1) (Fig. 1) contains one monomeric octa-coordinated strontium complex cation, $[\text{Sr}(\text{C}_3\text{H}_7\text{NO}_2)_4]^{2+}$, and two Br^- anions. In the cation, the Sr atom lies on a twofold axis and is surrounded by four *R*-lactamide ligands coordinated in a bidentate fashion *via* amide atom O1 (or O6) and hydroxy atom O2 (or O7) and their symmetry equivalents. The Sr coordination in the cation can be approximately described as a very distorted square antiprism arrangement [with square bases: O1 O2 O6ⁱ O7ⁱ and O1ⁱ O2ⁱ O6 O7; *i*: 1 - *x*, 1 - *y*, *z*] with the Sr atom shifted away from these (symmetry related) least-squares planes by 1.481 (2) Å. The Sr—O (amide) distances are similar within three estimated standard deviations [Sr—O1 (or O1ⁱ): 2.533 (3) and Sr—O6 (or O6ⁱ): 2.544 (4) Å]; among the Sr—O (hydroxy) distances Sr—O2 (or O2ⁱ): 2.535 (4) Å is equivalent to precedent values within three estimated standard deviations but very different from the two other distances Sr—O7 (or O7ⁱ): 2.703 (3) Å. All these values can be compared to those found in the poly[[tetaaquatris(monomethyl fumarato)distrontium(II)]monomethyl fumarate] in which the Sr atom is octa- coordinated by oxygen atoms which range from 2.499 (2) to 2.812 (2) Å (Stahl *et al.*, 2006). Among the two possible coordination modes (N,*O* or O,*O*) in metal complexes with lactamide or its derivatives described in the literature, the title compound presents the O,*O* mode like those in the complexes with the $[\text{Zn}(\text{lactamide})_3]^{2+}$ (Bekaert *et al.*, 2005) or the $[\text{B}(\text{lactamide})_2]^+$ (Bekaert *et al.*, 2007) cations.

The packing is charaterized by a number of H-bonds (Table 2). In particular, Br^- anions are linked to the cation by N—H \cdots Br and O—H \cdots Br hydrogen bonds, generating a three dimensional network.

Experimental

The title compound was prepared as follows: *S*-lactamide (0.356 g, 4 mmole) was dissolved in 20 ml of hot ethanol. Strontium dibromide (0.247 g, 1 mmole) was added to this solution with the help of an ultrasonic bath; the reaction medium was kept at 40° C for 48 h. Colourless plates of the title compound slowly appeared in the solution, whereupon crystals suitable for X-ray diffraction were obtained.

Refinement

H atoms except those bonded to hydroxy O atoms were positioned geometrically and refined using a riding model, with C—H = 0.96–0.98 Å and N—H = 0.86 Å with $U_{\text{iso}}(\text{H}) = 1.2$ (1.5 for methyl groups) times $U_{\text{eq}}(\text{C}, \text{O})$. H atoms bonded to hydroxy O atoms were located in a difference map and refined with an O—H distance restrained to 0.82 (1) Å and a common displacement parameter.

Figures

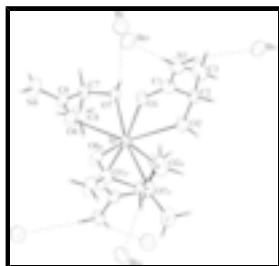


Fig. 1. Molecular view of the complex showing atomic numbering and some N—H...Br and O—H...Br hydrogen bonds in dotted lines. Displacement ellipsoids drawn at the 50% probability level. Symmetry codes: i: (1 - x, 1 - y, z), ii: (x + 1/2, 1/2 - y, -z) and iii: (x + 1/2, 1/2 - y, 1 - z).

Tetrakis[(*R*)-propionamide- $\kappa^2\text{O},\text{O}'$]strontium(II) dibromide

Crystal data

[Sr(C₃H₇NO₂)₄]Br₂

$M_r = 603.82$

Orthorhombic, $P2_12_12$

Hall symbol: P22ab

$a = 10.385$ (2) Å

$b = 17.919$ (2) Å

$c = 6.308$ (1) Å

$V = 1173.8$ (3) Å³

$Z = 2$

$F_{000} = 600$

$D_x = 1.708$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 3.2$ – 10.4°

$\mu = 5.74$ mm⁻¹

$T = 293$ (2) K

Parallelepiped, colourless

$0.25 \times 0.16 \times 0.12$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

ω – 2θ scans

Absorption correction: empirical (using intensity
measurements)

[multi-scan (Blessing, 1995)]

$T_{\text{min}} = 0.27$, $T_{\text{max}} = 0.50$

7106 measured reflections

$R_{\text{int}} = 0.067$

$\theta_{\text{max}} = 30.0^\circ$

$\theta_{\text{min}} = 2.3^\circ$

$h = -14 \rightarrow 14$

$k = 0 \rightarrow 25$

$l = 0 \rightarrow 8$

3 standard reflections

every 60 min

3407 independent reflections
2379 reflections with $I > 2\sigma(I)$

intensity decay: 1%

Refinement

Refinement on F^2

Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

H atoms treated by a mixture of independent and constrained refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$

$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2) = 0.111$

$(\Delta/\sigma)_{\max} < 0.001$

$S = 0.99$

$\Delta\rho_{\max} = 0.68 \text{ e } \text{\AA}^{-3}$

3407 reflections

$\Delta\rho_{\min} = -1.77 \text{ e } \text{\AA}^{-3}$

130 parameters

Extinction correction: none

2 restraints

Absolute structure: Flack (1983), 1415 Friedel pairs

Primary atom site location: structure-invariant direct methods

Flack parameter: $-0.017(15)$

Secondary atom site location: difference Fourier map

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	0.5000	0.5000	0.22123 (9)	0.02564 (14)
Br2	0.46507 (5)	0.22333 (3)	0.18621 (9)	0.04246 (16)
O1	0.6729 (4)	0.4010 (2)	0.1870 (6)	0.0382 (8)
N1	0.8257 (5)	0.3235 (3)	0.3141 (8)	0.0451 (11)
H1A	0.8500	0.3105	0.1891	0.054*
H1B	0.8631	0.3049	0.4237	0.054*
C1	0.7299 (5)	0.3726 (3)	0.3381 (9)	0.0339 (11)
O2	0.6163 (5)	0.4554 (2)	0.5510 (5)	0.0532 (12)
C2	0.6915 (5)	0.3896 (3)	0.5667 (8)	0.0358 (11)
H2	0.7692	0.4003	0.6494	0.043*
C3	0.6207 (6)	0.3266 (4)	0.6677 (10)	0.0531 (15)
H3A	0.5987	0.3398	0.8107	0.080*
H3B	0.6743	0.2830	0.6685	0.080*

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H3C	0.5435	0.3166	0.5889	0.080*
O6	0.3820 (4)	0.4505 (2)	−0.1029 (5)	0.0395 (8)
N6	0.2431 (5)	0.3752 (3)	−0.2688 (7)	0.0512 (13)
H6A	0.2706	0.3886	−0.3916	0.061*
H6B	0.1821	0.3429	−0.2586	0.061*
C6	0.2940 (5)	0.4038 (3)	−0.0976 (8)	0.0315 (10)
O7	0.3377 (3)	0.3834 (2)	0.2705 (6)	0.0310 (7)
C7	0.2392 (5)	0.3787 (3)	0.1129 (7)	0.0293 (10)
H7	0.2085	0.3271	0.1016	0.035*
C8	0.1284 (6)	0.4296 (4)	0.1775 (11)	0.0549 (16)
H8A	0.0944	0.4135	0.3114	0.082*
H8B	0.0619	0.4274	0.0720	0.082*
H8C	0.1592	0.4799	0.1899	0.082*
H2A	0.616 (6)	0.478 (3)	0.664 (5)	0.048 (13)*
H7A	0.377 (5)	0.3439 (18)	0.284 (10)	0.048 (13)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0258 (3)	0.0306 (3)	0.0205 (2)	−0.0015 (2)	0.000	0.000
Br2	0.0340 (3)	0.0484 (3)	0.0450 (3)	0.0041 (2)	0.0001 (2)	−0.0050 (2)
O1	0.046 (2)	0.046 (2)	0.0221 (17)	0.0127 (16)	0.0012 (16)	−0.0005 (15)
N1	0.045 (3)	0.055 (3)	0.036 (2)	0.021 (2)	0.009 (2)	0.000 (2)
C1	0.032 (3)	0.033 (3)	0.036 (3)	−0.003 (2)	0.005 (2)	0.001 (2)
O2	0.075 (3)	0.059 (3)	0.026 (2)	0.034 (2)	−0.0096 (19)	−0.0134 (18)
C2	0.039 (3)	0.042 (3)	0.027 (2)	0.013 (2)	−0.004 (2)	−0.004 (2)
C3	0.051 (3)	0.070 (4)	0.038 (3)	0.002 (3)	0.007 (3)	0.009 (3)
O6	0.043 (2)	0.050 (2)	0.0253 (16)	−0.0210 (18)	0.0001 (15)	0.0049 (16)
N6	0.053 (3)	0.074 (4)	0.027 (2)	−0.032 (3)	−0.001 (2)	0.003 (2)
C6	0.028 (3)	0.038 (3)	0.029 (2)	−0.002 (2)	−0.0001 (19)	0.000 (2)
O7	0.0345 (17)	0.0374 (18)	0.0212 (16)	−0.0033 (14)	−0.0022 (13)	0.0008 (14)
C7	0.030 (3)	0.036 (3)	0.022 (2)	−0.006 (2)	0.0018 (18)	0.0018 (18)
C8	0.033 (3)	0.079 (4)	0.053 (4)	0.005 (3)	0.007 (3)	−0.007 (3)

Geometric parameters (\AA , $^\circ$)

Sr1—O1 ⁱ	2.533 (3)	C2—H2	0.9800
Sr1—O1	2.533 (3)	C3—H3A	0.9600
Sr1—O2	2.535 (4)	C3—H3B	0.9600
Sr1—O2 ⁱ	2.535 (4)	C3—H3C	0.9600
Sr1—O6	2.544 (4)	O6—C6	1.239 (6)
Sr1—O6 ⁱ	2.544 (4)	N6—C6	1.307 (7)
Sr1—O7 ⁱ	2.703 (3)	N6—H6A	0.8600
Sr1—O7	2.703 (3)	N6—H6B	0.8600
O1—C1	1.232 (6)	C6—C7	1.513 (7)
N1—C1	1.337 (7)	O7—C7	1.429 (6)
N1—H1A	0.8600	O7—H7A	0.82 (4)
N1—H1B	0.8600	C7—C8	1.523 (7)

C1—C2	1.526 (7)	C7—H7	0.9800
O2—C2	1.417 (6)	C8—H8A	0.9600
O2—H2A	0.82 (4)	C8—H8B	0.9600
C2—C3	1.490 (8)	C8—H8C	0.9600
O1 ⁱ —Sr1—O1	170.23 (17)	C2—O2—H2A	111 (4)
O1 ⁱ —Sr1—O2	128.95 (12)	Sr1—O2—H2A	124 (4)
O1—Sr1—O2	60.74 (12)	O2—C2—C3	112.8 (5)
O1 ⁱ —Sr1—O2 ⁱ	60.74 (12)	O2—C2—C1	104.1 (4)
O1—Sr1—O2 ⁱ	128.95 (12)	C3—C2—C1	112.4 (5)
O2—Sr1—O2 ⁱ	69.71 (18)	O2—C2—H2	109.1
O1 ⁱ —Sr1—O6	80.46 (13)	C3—C2—H2	109.1
O1—Sr1—O6	91.65 (13)	C1—C2—H2	109.1
O2—Sr1—O6	141.18 (13)	C2—C3—H3A	109.5
O2 ⁱ —Sr1—O6	122.69 (15)	C2—C3—H3B	109.5
O1 ⁱ —Sr1—O6 ⁱ	91.65 (13)	H3A—C3—H3B	109.5
O1—Sr1—O6 ⁱ	80.46 (13)	C2—C3—H3C	109.5
O2—Sr1—O6 ⁱ	122.69 (15)	H3A—C3—H3C	109.5
O2 ⁱ —Sr1—O6 ⁱ	141.18 (13)	H3B—C3—H3C	109.5
O6—Sr1—O6 ⁱ	73.01 (15)	C6—O6—Sr1	124.7 (3)
O1 ⁱ —Sr1—O7 ⁱ	84.87 (12)	C6—N6—H6A	120.0
O1—Sr1—O7 ⁱ	96.26 (12)	C6—N6—H6B	120.0
O2—Sr1—O7 ⁱ	81.50 (13)	H6A—N6—H6B	120.0
O2 ⁱ —Sr1—O7 ⁱ	87.64 (14)	O6—C6—N6	122.7 (5)
O6—Sr1—O7 ⁱ	131.51 (11)	O6—C6—C7	120.1 (5)
O6 ⁱ —Sr1—O7 ⁱ	61.46 (11)	N6—C6—C7	117.1 (4)
O1 ⁱ —Sr1—O7	96.26 (12)	C7—O7—Sr1	114.3 (3)
O1—Sr1—O7	84.87 (12)	C7—O7—H7A	112 (5)
O2—Sr1—O7	87.64 (14)	Sr1—O7—H7A	112 (4)
O2 ⁱ —Sr1—O7	81.50 (13)	O7—C7—C6	108.9 (4)
O6—Sr1—O7	61.46 (11)	O7—C7—C8	108.6 (4)
O6 ⁱ —Sr1—O7	131.51 (11)	C6—C7—C8	109.9 (4)
O7 ⁱ —Sr1—O7	166.78 (15)	O7—C7—H7	109.8
C1—O1—Sr1	124.3 (3)	C6—C7—H7	109.8
C1—N1—H1A	120.0	C8—C7—H7	109.8
C1—N1—H1B	120.0	C7—C8—H8A	109.5
H1A—N1—H1B	120.0	C7—C8—H8B	109.5
O1—C1—N1	122.8 (5)	H8A—C8—H8B	109.5
O1—C1—C2	121.5 (5)	C7—C8—H8C	109.5
N1—C1—C2	115.6 (5)	H8A—C8—H8C	109.5
C2—O2—Sr1	125.6 (3)	H8B—C8—H8C	109.5

Symmetry codes: (i) $-x+1, -y+1, z$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O7-H7A\cdots Br2$	0.82 (4)	2.43 (3)	3.203 (4)	158 (6)
$N1-H1A\cdots Br2^{ii}$	0.86	2.72	3.572 (5)	171
$N1-H1B\cdots Br2^{iii}$	0.86	2.73	3.568 (5)	167
$O2-H2A\cdots O6^{iv}$	0.82 (4)	1.95 (4)	2.759 (5)	169 (6)
$N6-H6A\cdots O7^v$	0.86	2.24	3.071 (6)	161
$N6-H6B\cdots Br2^{vi}$	0.86	2.59	3.424 (5)	164

Symmetry codes: (ii) $x+1/2, -y+1/2, -z$; (iii) $x+1/2, -y+1/2, -z+1$; (iv) $-x+1, -y+1, z+1$; (v) $x, y, z-1$; (vi) $x-1/2, -y+1/2, -z$.

Fig. 1

