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Strontium nitride carbodiimide, $Sr_4N_2(CN_2)$

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(N–C) = 0.006 Å
R factor = 0.026
wR factor = 0.050
Data-to-parameter ratio = 20.6

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

Strontium nitride carbodiimide, $Sr_4N_2(CN_2)$, is isostructural with the calcium analogue and consists of a framework of edge- and vertex-sharing Sr_6N octahedra forming channels within which almost linear and almost symmetrical carbodiimide anions reside, surrounded by eight strontium ions.

Comment

There is increasing interest in the chemistry of the nitrides of the elements and one way to grow crystals of alkaline earth main group nitrides is to make use of a molten sodium flux (Yamane & DiSalvo, 1996; Reckeweg & DiSalvo, 2000). In attempting to grow crystals of strontium aluminium nitrides we grew crystals of the title phase. Strontium nitride carbodiimide is isostructural with the calcium analogue $Ca_4N_2(CN_2)$ (Reckeweg & DiSalvo, 2000) and with $Ca_{3.2}Sr_{0.8}N_2(CN_2)$ (Höhn *et al.*, 2000). The structure consists of a three-dimensional framework of Sr_6N octahedra, centred by atoms N3 and N4, linked by their edges and vertices. Channels are formed which accommodate the carbodiimide anions. Each N atom of the carbodiimide anion is within 3.0 Å of four strontium ions and the $[CN_2]^{2-}$ anions should be considered eight-coordinate by strontium cations. Atoms Sr1 and Sr3 are coordinated by five N atoms within 3 Å, Sr2 is in approximately octahedral coordination by six N atoms, and Sr4 is in distorted tetrahedral coordination by four N atoms within 2.7 Å, with a fifth N atom 3.228 (4) Å distant. The carbodiimide anions are almost linear, with an N—C—N bond angle of 178.0 (5)°, and the anion is in the symmetrical carbodiimide form, with C—N bond lengths of 1.240 (6) and 1.235 (6) Å, which are equal within experi-

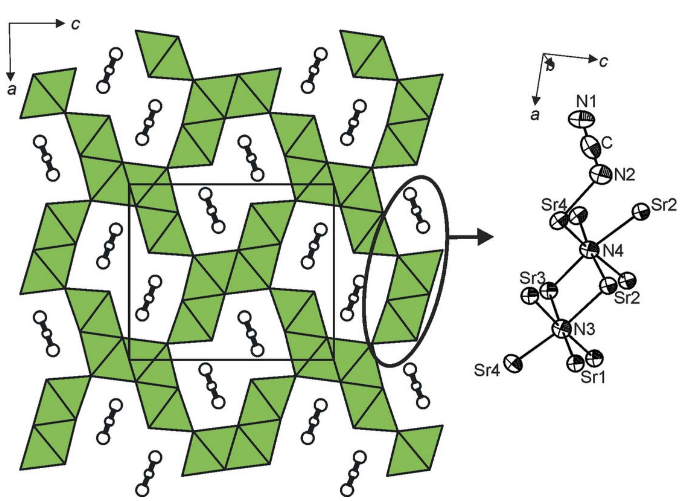

Figure 1
The structure of $Sr_4N_2(CN_2)$, showing the framework of Sr_6N octahedra and the channels containing the carbodiimide anions. The detail shows the asymmetric unit, with 99% displacement ellipsoids.

mental uncertainty. The geometry of the carbodiimide anions in $Ca_4N_2(CN_2)$ is similar: C—N bond lengths of 1.22 (1) and 1.24 (1) Å, and an N—C—N angle of 179.7 (10)° (Reckeweg & DiSalvo, 2000). The structure of $Sr_4N_2(CN_2)$ is shown in Fig. 1.

Experimental

Strontium nitride carbodiimide was synthesized by reacting together Sr (99%, Aldrich, 100 mg), NaN_3 (99%, Aldrich, 85 mg), Al (99.99%, Aldrich, 31 mg) and Na (99+ %, BDH, 200 mg) in a sealed nickel tube at 1073 K for 4 d, with slow cooling to 673 K prior to removal of the tube from the furnace. A small number of colourless crystals of the product were obtained after sublimation of excess sodium from the reactants. No other crystalline products were identified in the reaction. The carbon forming the carbodiimide units presumably arises adventitiously from the nickel tube or from one or more of the reactants, as noted by Reckeweg & DiSalvo (2000).

Crystal data

$Sr_4N_2(CN_2)$
M_r = 418.53
Orthorhombic, *Pnma*
a = 12.2928 (4) Å
b = 3.8261 (1) Å
c = 14.3291 (5) Å
V = 673.95 (4) Å^3
Z = 4
D_x = 4.125 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 43855 reflections
θ = 1.0–33.1°
μ = 31.39 mm^{-1}
T = 150 (2) K
Prism, colourless above
0.09 × 0.05 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: analytical (Alcock, 1970)
T_{min} = 0.062, T_{max} = 0.301
14693 measured reflections
1156 independent reflections
942 reflections with $I > 2\sigma(I)$
R_{int} = 0.076
θ_{max} = 30.5°
$h = -17 \rightarrow 17$
$k = -5 \rightarrow 5$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.050
S = 1.07
1156 reflections
56 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0142P)^2 + 1.6092P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.99 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.00093 (15)

Table 1
Selected geometric parameters (Å, °).

Sr1—N3^{i}	2.551 (3)	Sr3—N4	2.490 (4)
Sr1—N3^{ii}	2.551 (3)	Sr3—N3^{ii}	2.616 (3)
Sr1—N2	2.799 (4)	Sr3—N3^{i}	2.616 (3)
Sr1—N1^{iii}	2.837 (3)	Sr3—N1^{i}	2.998 (3)
Sr1—N1^{iv}	2.837 (3)	Sr3—N1^{ii}	2.998 (3)
Sr2—N4^{v}	2.674 (3)	Sr4—N4^{viii}	2.500 (2)
Sr2—N4^{vi}	2.674 (3)	Sr4—N4^{ix}	2.500 (2)
Sr2—N3	2.740 (4)	Sr4—N3	2.592 (4)
Sr2—N4^{vii}	2.774 (4)	Sr4—N2	2.683 (4)
Sr2—N2^{vi}	2.867 (3)	N1—C5	1.240 (6)
Sr2—N2^{v}	2.867 (3)	N2—C5	1.235 (6)
N2—C5—N1	178.0 (5)		

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

The highest residdual electron-density peak is located 1.57 Å from atom Sr3. [1.12 e Å^{-3}].

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELX97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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supporting information

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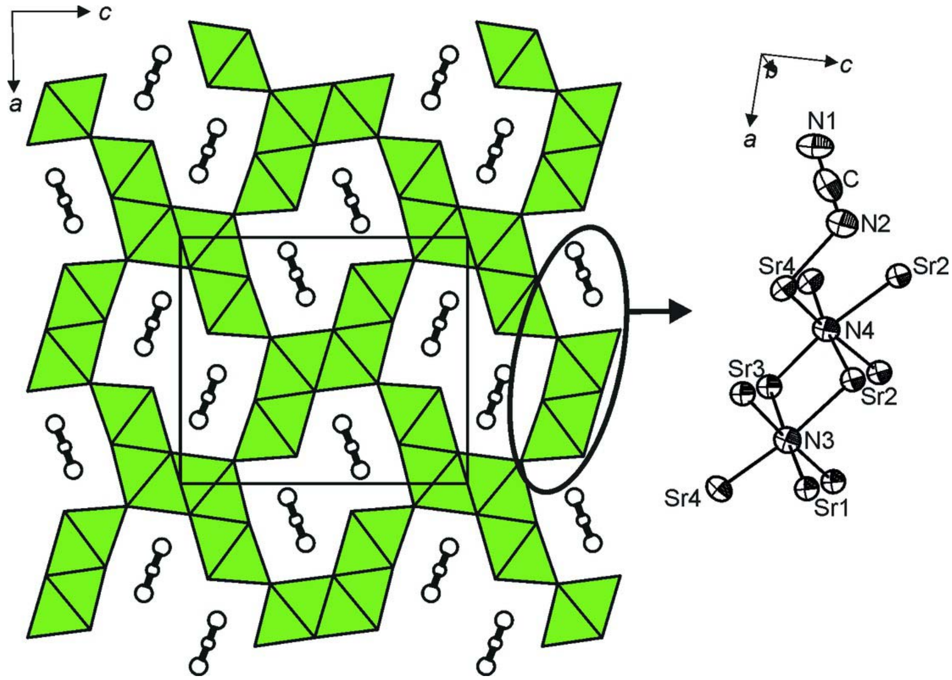

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Strontium nitride carbodiimide

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Hall symbol: -P 2ac 2n
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c = 14.3291 (5) Å
V = 673.95 (4) Å^3
Z = 4
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D_x = 4.125 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 43855 reflections
θ = 1.0–33.1°
μ = 31.39 mm^{-1}
T = 150 K
Prism, white
0.09 × 0.05 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: Enraf Nonius FR590
Graphite monochromator
CCD rotation images, thick slices scans
Absorption correction: analytical (Alcock, 1970)
T_{min} = 0.062, T_{max} = 0.301
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1156 independent reflections
942 reflections with $I > 2\sigma(I)$
R_{int} = 0.076
θ_{max} = 30.5°, θ_{min} = 5.2°
$h = -17 \rightarrow 17$
$k = -5 \rightarrow 5$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.050$
$S = 1.07$
1156 reflections
56 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0142P)^2 + 1.6092P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.12$ e Å^{-3}
$\Delta\rho_{min} = -0.99$ e Å^{-3}
Extinction correction: *SHELXL97*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00093 (15)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Sr1	0.11185 (3)	0.25	0.59628 (3)	0.00995 (11)
Sr2	0.12505 (3)	0.25	0.03205 (3)	0.00994 (11)
Sr3	0.33905 (3)	0.25	0.73997 (3)	0.00994 (11)
Sr4	0.40728 (3)	0.25	0.31366 (3)	0.01062 (11)
N1	0.0547 (3)	0.25	0.3728 (3)	0.0178 (9)
N2	0.2420 (3)	0.25	0.4360 (3)	0.0164 (9)
N3	0.2803 (3)	0.25	0.1692 (3)	0.0115 (8)
N4	0.4864 (3)	0.25	0.6207 (3)	0.0115 (8)
C5	0.1492 (4)	0.25	0.4031 (4)	0.0144 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0104 (2)	0.00829 (19)	0.0111 (2)	0	−0.00008 (16)	0
Sr2	0.0105 (2)	0.00805 (19)	0.0112 (2)	0	0.00027 (16)	0
Sr3	0.0103 (2)	0.00786 (18)	0.0117 (2)	0	−0.00007 (16)	0
Sr4	0.0118 (2)	0.00723 (19)	0.0128 (2)	0	−0.00272 (17)	0
N1	0.0107 (19)	0.0163 (19)	0.026 (2)	0	0.0005 (18)	0
N2	0.014 (2)	0.0161 (19)	0.019 (2)	0	0.0015 (17)	0
N3	0.0130 (19)	0.0081 (17)	0.014 (2)	0	−0.0004 (16)	0
N4	0.0109 (18)	0.0096 (17)	0.014 (2)	0	0.0006 (15)	0
C5	0.020 (2)	0.0086 (19)	0.015 (2)	0	0.005 (2)	0

Geometric parameters (Å, º)

Sr1—N3^{i}	2.551 (3)	Sr3—Sr4^{i}	3.7341 (5)
Sr1—N3^{ii}	2.551 (3)	Sr4—N4^{xi}	2.500 (2)
Sr1—N2	2.799 (4)	Sr4—N4^{xii}	2.500 (2)
Sr1—C5	2.807 (5)	Sr4—N3	2.592 (4)
Sr1—N1^{iii}	2.837 (3)	Sr4—N2	2.683 (4)
Sr1—N1^{iv}	2.837 (3)	Sr4—N1^{xiii}	3.228 (4)
Sr1—N1	3.279 (5)	Sr4—Sr2^{xiii}	3.4720 (6)
Sr1—Sr3	3.4699 (6)	Sr4—Sr1^{vii}	3.6629 (5)
Sr1—Sr4^{i}	3.6629 (5)	Sr4—Sr1^{viii}	3.6629 (5)
Sr1—Sr4^{ii}	3.6629 (5)	Sr4—Sr2^{i}	3.6893 (5)
Sr1—Sr1^{v}	3.8261 (1)	Sr4—Sr2^{ii}	3.6893 (5)
Sr1—Sr1^{vi}	3.8261 (1)	Sr4—Sr3^{vii}	3.7341 (5)
Sr2—N4^{vii}	2.674 (3)	Sr4—Sr3^{viii}	3.7341 (5)
Sr2—N4^{viii}	2.674 (3)	N1—C5	1.240 (6)
Sr2—N3	2.740 (4)	N1—Sr1^{iii}	2.837 (3)
Sr2—N4^{ix}	2.774 (4)	N1—Sr1^{iv}	2.837 (3)
Sr2—N2^{viii}	2.867 (3)	N1—Sr3^{vii}	2.998 (3)
Sr2—N2^{vii}	2.867 (3)	N1—Sr3^{viii}	2.998 (3)
Sr2—Sr4^{ix}	3.4720 (6)	N1—Sr4^{ix}	3.228 (4)
Sr2—Sr3^{viii}	3.5680 (5)	N2—C5	1.235 (6)
Sr2—Sr3^{vii}	3.5680 (5)	N2—Sr2^{i}	2.867 (3)
Sr2—Sr4^{vii}	3.6893 (5)	N2—Sr2^{ii}	2.867 (3)
Sr2—Sr4^{viii}	3.6893 (5)	N3—Sr1^{viii}	2.551 (3)
Sr2—Sr2^{x}	3.7358 (7)	N3—Sr1^{vii}	2.551 (3)
Sr3—N4	2.490 (4)	N3—Sr3^{vii}	2.616 (3)
Sr3—N3^{ii}	2.616 (3)	N3—Sr3^{viii}	2.616 (3)
Sr3—N3^{i}	2.616 (3)	N4—Sr4^{xi}	2.500 (2)
Sr3—N1^{i}	2.998 (3)	N4—Sr4^{xii}	2.500 (2)
Sr3—N1^{ii}	2.998 (3)	N4—Sr2^{ii}	2.674 (3)
Sr3—C5^{i}	3.024 (4)	N4—Sr2^{i}	2.674 (3)
Sr3—C5^{ii}	3.024 (4)	N4—Sr2^{xiii}	2.774 (4)
Sr3—Sr2^{ii}	3.5680 (5)	C5—Sr3^{vii}	3.024 (4)
Sr3—Sr2^{i}	3.5680 (5)	C5—Sr3^{viii}	3.024 (4)
Sr3—Sr4^{ii}	3.7341 (5)		
N3^{i}—Sr1—N3^{ii}	97.16 (13)	N4—Sr3—Sr2^{i}	48.48 (6)
N3^{i}—Sr1—N2	92.24 (10)	N3^{ii}—Sr3—Sr2^{i}	97.93 (8)
N3^{ii}—Sr1—N2	92.24 (10)	N3^{i}—Sr3—Sr2^{i}	49.73 (9)
N3^{i}—Sr1—C5	108.62 (11)	N1^{i}—Sr3—Sr2^{i}	97.70 (7)
N3^{ii}—Sr1—C5	108.62 (11)	N1^{ii}—Sr3—Sr2^{i}	144.92 (8)
N2—Sr1—C5	25.46 (13)	C5^{i}—Sr3—Sr2^{i}	107.47 (6)
N3^{i}—Sr1—N1^{iii}	144.73 (12)	C5^{ii}—Sr3—Sr2^{i}	168.16 (9)
N3^{ii}—Sr1—N1^{iii}	78.77 (10)	Sr1—Sr3—Sr2^{i}	66.676 (11)
N2—Sr1—N1^{iii}	122.75 (10)	Sr2^{ii}—Sr3—Sr2^{i}	64.846 (11)
C5—Sr1—N1^{iii}	105.80 (11)	N4—Sr3—Sr4^{ii}	141.62 (5)
N3^{i}—Sr1—N1^{iv}	78.77 (10)	N3^{ii}—Sr3—Sr4^{ii}	43.93 (9)

N3^{ii}—Sr1—N1^{iv}	144.73 (12)	N3^{i}—Sr3—Sr4^{ii}	91.68 (8)
N2—Sr1—N1^{iv}	122.75 (10)	N1^{i}—Sr3—Sr4^{ii}	120.05 (8)
C5—Sr1—N1^{iv}	105.80 (11)	N1^{ii}—Sr3—Sr4^{ii}	81.19 (7)
N1^{iii}—Sr1—N1^{iv}	84.80 (11)	C5^{i}—Sr3—Sr4^{ii}	98.30 (9)
N3^{i}—Sr1—N1	120.76 (9)	C5^{ii}—Sr3—Sr4^{ii}	59.74 (9)
N3^{ii}—Sr1—N1	120.76 (9)	Sr1—Sr3—Sr4^{ii}	60.992 (11)
N2—Sr1—N1	47.24 (11)	Sr2^{ii}—Sr3—Sr4^{ii}	93.538 (10)
C5—Sr1—N1	21.78 (12)	Sr2^{i}—Sr3—Sr4^{ii}	127.667 (15)
N1^{iii}—Sr1—N1	89.89 (11)	N4—Sr3—Sr4^{i}	141.62 (5)
N1^{iv}—Sr1—N1	89.89 (11)	N3^{ii}—Sr3—Sr4^{i}	91.68 (8)
N3^{i}—Sr1—Sr3	48.61 (7)	N3^{i}—Sr3—Sr4^{i}	43.93 (9)
N3^{ii}—Sr1—Sr3	48.61 (7)	N1^{i}—Sr3—Sr4^{i}	81.19 (7)
N2—Sr1—Sr3	91.52 (9)	N1^{ii}—Sr3—Sr4^{i}	120.05 (8)
C5—Sr1—Sr3	116.98 (10)	C5^{i}—Sr3—Sr4^{i}	59.74 (9)
N1^{iii}—Sr1—Sr3	119.22 (8)	C5^{ii}—Sr3—Sr4^{i}	98.30 (9)
N1^{iv}—Sr1—Sr3	119.22 (8)	Sr1—Sr3—Sr4^{i}	60.992 (11)
N1—Sr1—Sr3	138.77 (7)	Sr2^{ii}—Sr3—Sr4^{i}	127.667 (15)
N3^{i}—Sr1—Sr4^{i}	45.03 (9)	Sr2^{i}—Sr3—Sr4^{i}	93.538 (10)
N3^{ii}—Sr1—Sr4^{i}	94.39 (8)	Sr4^{ii}—Sr3—Sr4^{i}	61.636 (9)
N2—Sr1—Sr4^{i}	137.25 (6)	N4^{xi}—Sr4—N4^{xii}	99.84 (13)
C5—Sr1—Sr4^{i}	148.147 (16)	N4^{xi}—Sr4—N3	127.95 (7)
N1^{iii}—Sr1—Sr4^{i}	99.96 (8)	N4^{xii}—Sr4—N3	127.95 (7)
N1^{iv}—Sr1—Sr4^{i}	57.90 (9)	N4^{xi}—Sr4—N2	98.62 (11)
N1—Sr1—Sr4^{i}	144.77 (3)	N4^{xii}—Sr4—N2	98.62 (11)
Sr3—Sr1—Sr4^{i}	63.069 (11)	N3—Sr4—N2	93.79 (12)
N3^{i}—Sr1—Sr4^{ii}	94.39 (8)	N4^{xi}—Sr4—N1^{xiii}	91.02 (10)
N3^{ii}—Sr1—Sr4^{ii}	45.03 (9)	N4^{xii}—Sr4—N1^{xiii}	91.02 (10)
N2—Sr1—Sr4^{ii}	137.25 (6)	N3—Sr4—N1^{xiii}	71.17 (12)
C5—Sr1—Sr4^{ii}	148.147 (16)	N2—Sr4—N1^{xiii}	164.96 (12)
N1^{iii}—Sr1—Sr4^{ii}	57.90 (9)	N4^{xi}—Sr4—Sr2^{xiii}	50.03 (7)
N1^{iv}—Sr1—Sr4^{ii}	99.96 (8)	N4^{xii}—Sr4—Sr2^{xiii}	50.03 (7)
N1—Sr1—Sr4^{ii}	144.77 (3)	N3—Sr4—Sr2^{xiii}	166.57 (9)
Sr3—Sr1—Sr4^{ii}	63.069 (11)	N2—Sr4—Sr2^{xiii}	99.65 (9)
Sr4^{i}—Sr1—Sr4^{ii}	62.969 (10)	N1^{xiii}—Sr4—Sr2^{xiii}	95.39 (8)
N3^{i}—Sr1—Sr1^{v}	41.42 (7)	N4^{xi}—Sr4—Sr1^{vii}	138.85 (9)
N3^{ii}—Sr1—Sr1^{v}	138.58 (7)	N4^{xii}—Sr4—Sr1^{vii}	87.35 (8)
N2—Sr1—Sr1^{v}	90	N3—Sr4—Sr1^{vii}	44.14 (6)
C5—Sr1—Sr1^{v}	90	N2—Sr4—Sr1^{vii}	120.47 (7)
N1^{iii}—Sr1—Sr1^{v}	132.40 (6)	N1^{xiii}—Sr4—Sr1^{vii}	48.12 (5)
N1^{iv}—Sr1—Sr1^{v}	47.60 (6)	Sr2^{xiii}—Sr4—Sr1^{vii}	126.227 (13)
N1—Sr1—Sr1^{v}	90	N4^{xi}—Sr4—Sr1^{viii}	87.35 (8)
Sr3—Sr1—Sr1^{v}	90	N4^{xii}—Sr4—Sr1^{viii}	138.85 (9)
Sr4^{i}—Sr1—Sr1^{v}	58.515 (5)	N3—Sr4—Sr1^{viii}	44.14 (6)
Sr4^{ii}—Sr1—Sr1^{v}	121.485 (5)	N2—Sr4—Sr1^{viii}	120.47 (7)
N3^{i}—Sr1—Sr1^{vi}	138.58 (7)	N1^{xiii}—Sr4—Sr1^{viii}	48.12 (5)
N3^{ii}—Sr1—Sr1^{vi}	41.42 (7)	Sr2^{xiii}—Sr4—Sr1^{viii}	126.227 (13)
N2—Sr1—Sr1^{vi}	90	Sr1^{vii}—Sr4—Sr1^{viii}	62.970 (10)
C5—Sr1—Sr1^{vi}	90	N4^{xi}—Sr4—Sr2^{i}	48.74 (9)

N1^{iii}—Sr1—Sr1^{vi}	47.60 (6)
N1^{iv}—Sr1—Sr1^{vi}	132.40 (6)
N1—Sr1—Sr1^{vi}	90
Sr3—Sr1—Sr1^{vi}	90
Sr4^{i}—Sr1—Sr1^{vi}	121.485 (5)
Sr4^{ii}—Sr1—Sr1^{vi}	58.515 (5)
Sr1^{v}—Sr1—Sr1^{vi}	180.00 (2)
N4^{vii}—Sr2—N4^{viii}	91.34 (12)
N4^{vii}—Sr2—N3	90.93 (10)
N4^{viii}—Sr2—N3	90.93 (10)
N4^{vii}—Sr2—N4^{ix}	93.45 (10)
N4^{viii}—Sr2—N4^{ix}	93.45 (10)
N3—Sr2—N4^{ix}	173.73 (11)
N4^{vii}—Sr2—N2^{viii}	175.70 (9)
N4^{viii}—Sr2—N2^{viii}	92.45 (8)
N3—Sr2—N2^{viii}	86.98 (10)
N4^{ix}—Sr2—N2^{viii}	88.36 (10)
N4^{vii}—Sr2—N2^{vii}	92.45 (8)
N4^{viii}—Sr2—N2^{vii}	175.70 (9)
N3—Sr2—N2^{vii}	86.98 (10)
N4^{ix}—Sr2—N2^{vii}	88.36 (10)
N2^{viii}—Sr2—N2^{vii}	83.70 (11)
N4^{vii}—Sr2—Sr4^{ix}	45.76 (6)
N4^{viii}—Sr2—Sr4^{ix}	45.76 (6)
N3—Sr2—Sr4^{ix}	94.61 (8)
N4^{ix}—Sr2—Sr4^{ix}	91.65 (8)
N2^{viii}—Sr2—Sr4^{ix}	138.15 (6)
N2^{vii}—Sr2—Sr4^{ix}	138.15 (6)
N4^{vii}—Sr2—Sr3^{viii}	92.88 (7)
N4^{viii}—Sr2—Sr3^{viii}	44.21 (8)
N3—Sr2—Sr3^{viii}	46.75 (6)
N4^{ix}—Sr2—Sr3^{viii}	137.30 (5)
N2^{viii}—Sr2—Sr3^{viii}	88.43 (7)
N2^{vii}—Sr2—Sr3^{viii}	133.47 (8)
Sr4^{ix}—Sr2—Sr3^{viii}	64.129 (11)
N4^{vii}—Sr2—Sr3^{vii}	44.21 (8)
N4^{viii}—Sr2—Sr3^{vii}	92.88 (7)
N3—Sr2—Sr3^{vii}	46.75 (6)
N4^{ix}—Sr2—Sr3^{vii}	137.30 (5)
N2^{viii}—Sr2—Sr3^{vii}	133.47 (8)
N2^{vii}—Sr2—Sr3^{vii}	88.43 (7)
Sr4^{ix}—Sr2—Sr3^{vii}	64.129 (11)
Sr3^{viii}—Sr2—Sr3^{vii}	64.846 (11)
N4^{vii}—Sr2—Sr4^{vii}	88.67 (7)
N4^{viii}—Sr2—Sr4^{vii}	135.95 (8)
N3—Sr2—Sr4^{vii}	133.12 (6)
N4^{ix}—Sr2—Sr4^{vii}	42.65 (5)
N2^{viii}—Sr2—Sr4^{vii}	90.02 (7)
N4^{xii}—Sr4—Sr2^{i}	97.70 (8)
N3—Sr4—Sr2^{i}	127.77 (7)
N2—Sr4—Sr2^{i}	50.52 (7)
N1^{xiii}—Sr4—Sr2^{i}	139.68 (5)
Sr2^{xiii}—Sr4—Sr2^{i}	62.802 (12)
Sr1^{vii}—Sr4—Sr2^{i}	170.134 (16)
Sr1^{viii}—Sr4—Sr2^{i}	116.332 (6)
N4^{xi}—Sr4—Sr2^{ii}	97.70 (8)
N4^{xii}—Sr4—Sr2^{ii}	48.74 (9)
N3—Sr4—Sr2^{ii}	127.77 (7)
N2—Sr4—Sr2^{ii}	50.52 (7)
N1^{xiii}—Sr4—Sr2^{ii}	139.68 (5)
Sr2^{xiii}—Sr4—Sr2^{ii}	62.802 (12)
Sr1^{vii}—Sr4—Sr2^{ii}	116.332 (6)
Sr1^{viii}—Sr4—Sr2^{ii}	170.134 (16)
Sr2^{i}—Sr4—Sr2^{ii}	62.469 (10)
N4^{xi}—Sr4—Sr3^{vii}	157.24 (8)
N4^{xii}—Sr4—Sr3^{vii}	97.94 (7)
N3—Sr4—Sr3^{vii}	44.44 (6)
N2—Sr4—Sr3^{vii}	64.59 (7)
N1^{xiii}—Sr4—Sr3^{vii}	102.79 (7)
Sr2^{xiii}—Sr4—Sr3^{vii}	143.640 (9)
Sr1^{vii}—Sr4—Sr3^{vii}	55.940 (10)
Sr1^{viii}—Sr4—Sr3^{vii}	88.571 (12)
Sr2^{i}—Sr4—Sr3^{vii}	114.717 (14)
Sr2^{ii}—Sr4—Sr3^{vii}	83.502 (11)
N4^{xi}—Sr4—Sr3^{viii}	97.94 (7)
N4^{xii}—Sr4—Sr3^{viii}	157.24 (8)
N3—Sr4—Sr3^{viii}	44.44 (6)
N2—Sr4—Sr3^{viii}	64.59 (7)
N1^{xiii}—Sr4—Sr3^{viii}	102.79 (7)
Sr2^{xiii}—Sr4—Sr3^{viii}	143.640 (9)
Sr1^{vii}—Sr4—Sr3^{viii}	88.571 (12)
Sr1^{viii}—Sr4—Sr3^{viii}	55.940 (10)
Sr2^{i}—Sr4—Sr3^{viii}	83.502 (11)
Sr2^{ii}—Sr4—Sr3^{viii}	114.717 (14)
Sr3^{vii}—Sr4—Sr3^{viii}	61.636 (9)
C5—N1—Sr1^{iii}	128.41 (19)
C5—N1—Sr1^{iv}	128.41 (19)
Sr1^{iii}—N1—Sr1^{iv}	84.80 (11)
C5—N1—Sr3^{vii}	79.3 (2)
Sr1^{iii}—N1—Sr3^{vii}	89.04 (5)
Sr1^{iv}—N1—Sr3^{vii}	147.56 (17)
C5—N1—Sr3^{viii}	79.3 (2)
Sr1^{iii}—N1—Sr3^{viii}	147.56 (17)
Sr1^{iv}—N1—Sr3^{viii}	89.04 (5)
Sr3^{vii}—N1—Sr3^{viii}	79.31 (11)
C5—N1—Sr4^{ix}	144.7 (4)

N2^{vii}—Sr2—Sr4^{vii}	46.24 (8)	Sr1^{iii}—N1—Sr4^{ix}	73.99 (9)
Sr4^{ix}—Sr2—Sr4^{vii}	117.198 (12)	Sr1^{iv}—N1—Sr4^{ix}	73.99 (9)
Sr3^{viii}—Sr2—Sr4^{vii}	178.441 (13)	Sr3^{vii}—N1—Sr4^{ix}	73.70 (9)
Sr3^{vii}—Sr2—Sr4^{vii}	116.332 (6)	Sr3^{viii}—N1—Sr4^{ix}	73.70 (9)
N4^{vii}—Sr2—Sr4^{viii}	135.95 (8)	C5—N1—Sr1	57.1 (3)
N4^{viii}—Sr2—Sr4^{viii}	88.67 (7)	Sr1^{iii}—N1—Sr1	90.11 (11)
N3—Sr2—Sr4^{viii}	133.12 (6)	Sr1^{iv}—N1—Sr1	90.11 (11)
N4^{ix}—Sr2—Sr4^{viii}	42.65 (5)	Sr3^{vii}—N1—Sr1	121.78 (10)
N2^{viii}—Sr2—Sr4^{viii}	46.24 (8)	Sr3^{viii}—N1—Sr1	121.78 (10)
N2^{vii}—Sr2—Sr4^{viii}	90.02 (7)	Sr4^{ix}—N1—Sr1	158.21 (14)
Sr4^{ix}—Sr2—Sr4^{viii}	117.198 (12)	C5—N2—Sr4	116.7 (3)
Sr3^{viii}—Sr2—Sr4^{viii}	116.332 (6)	C5—N2—Sr1	77.6 (3)
Sr3^{vii}—Sr2—Sr4^{viii}	178.441 (13)	Sr4—N2—Sr1	165.68 (17)
Sr4^{vii}—Sr2—Sr4^{viii}	62.469 (10)	C5—N2—Sr2^{i}	135.23 (12)
N4^{vii}—Sr2—Sr2^{x}	47.84 (8)	Sr4—N2—Sr2^{i}	83.24 (10)
N4^{viii}—Sr2—Sr2^{x}	93.52 (7)	Sr1—N2—Sr2^{i}	86.11 (10)
N3—Sr2—Sr2^{x}	138.57 (5)	C5—N2—Sr2^{ii}	135.23 (12)
N4^{ix}—Sr2—Sr2^{x}	45.61 (6)	Sr4—N2—Sr2^{ii}	83.24 (10)
N2^{viii}—Sr2—Sr2^{x}	133.83 (8)	Sr1—N2—Sr2^{ii}	86.11 (10)
N2^{vii}—Sr2—Sr2^{x}	90.53 (7)	Sr2^{i}—N2—Sr2^{ii}	83.70 (11)
Sr4^{ix}—Sr2—Sr2^{x}	61.445 (13)	Sr1^{viii}—N3—Sr1^{vii}	97.16 (13)
Sr3^{viii}—Sr2—Sr2^{x}	125.567 (19)	Sr1^{viii}—N3—Sr4	90.83 (11)
Sr3^{vii}—Sr2—Sr2^{x}	91.864 (12)	Sr1^{vii}—N3—Sr4	90.83 (11)
Sr4^{vii}—Sr2—Sr2^{x}	55.753 (12)	Sr1^{viii}—N3—Sr3^{vii}	177.10 (16)
Sr4^{viii}—Sr2—Sr2^{x}	88.184 (16)	Sr1^{vii}—N3—Sr3^{vii}	84.366 (11)
N4—Sr3—N3^{ii}	98.18 (10)	Sr4—N3—Sr3^{vii}	91.62 (11)
N4—Sr3—N3^{i}	98.18 (10)	Sr1^{viii}—N3—Sr3^{viii}	84.366 (11)
N3^{ii}—Sr3—N3^{i}	94.01 (13)	Sr1^{vii}—N3—Sr3^{viii}	177.10 (16)
N4—Sr3—N1^{i}	96.81 (11)	Sr4—N3—Sr3^{viii}	91.62 (11)
N3^{ii}—Sr3—N1^{i}	163.18 (11)	Sr3^{vii}—N3—Sr3^{viii}	94.01 (13)
N3^{i}—Sr3—N1^{i}	91.36 (9)	Sr1^{viii}—N3—Sr2	93.90 (11)
N4—Sr3—N1^{ii}	96.81 (11)	Sr1^{vii}—N3—Sr2	93.90 (11)
N3^{ii}—Sr3—N1^{ii}	91.36 (9)	Sr4—N3—Sr2	172.85 (17)
N3^{i}—Sr3—N1^{ii}	163.18 (11)	Sr3^{vii}—N3—Sr2	83.52 (10)
N1^{i}—Sr3—N1^{ii}	79.31 (11)	Sr3^{viii}—N3—Sr2	83.52 (10)
N4—Sr3—C5^{i}	119.71 (11)	Sr3—N4—Sr4^{xi}	97.01 (11)
N3^{ii}—Sr3—C5^{i}	142.10 (13)	Sr3—N4—Sr4^{xii}	97.01 (11)
N3^{i}—Sr3—C5^{i}	82.16 (10)	Sr4^{xi}—N4—Sr4^{xii}	99.84 (13)
N1^{i}—Sr3—C5^{i}	23.76 (12)	Sr3—N4—Sr2^{ii}	87.32 (10)
N1^{ii}—Sr3—C5^{i}	83.82 (9)	Sr4^{xi}—N4—Sr2^{ii}	173.62 (16)
N4—Sr3—C5^{ii}	119.71 (11)	Sr4^{xii}—N4—Sr2^{ii}	84.211 (15)
N3^{ii}—Sr3—C5^{ii}	82.16 (10)	Sr3—N4—Sr2^{i}	87.32 (10)
N3^{i}—Sr3—C5^{ii}	142.10 (13)	Sr4^{xi}—N4—Sr2^{i}	84.211 (15)
N1^{i}—Sr3—C5^{ii}	83.82 (9)	Sr4^{xii}—N4—Sr2^{i}	173.62 (16)
N1^{ii}—Sr3—C5^{ii}	23.76 (12)	Sr2^{ii}—N4—Sr2^{i}	91.34 (12)
C5^{i}—Sr3—C5^{ii}	78.50 (12)	Sr3—N4—Sr2^{xiii}	171.22 (17)
N4—Sr3—Sr1	100.28 (9)	Sr4^{xi}—N4—Sr2^{xiii}	88.61 (10)
N3^{ii}—Sr3—Sr1	47.03 (6)	Sr4^{xii}—N4—Sr2^{xiii}	88.61 (10)

N3^{i}—Sr3—Sr1	47.03 (6)	Sr2^{ii}—N4—Sr2^{xiii}	86.55 (10)
N1^{i}—Sr3—Sr1	136.66 (6)	Sr2^{i}—N4—Sr2^{xiii}	86.55 (10)
N1^{ii}—Sr3—Sr1	136.66 (6)	N2—C5—N1	178.0 (5)
C5^{i}—Sr3—Sr1	119.81 (9)	N2—C5—Sr1	76.9 (3)
C5^{ii}—Sr3—Sr1	119.81 (9)	N1—C5—Sr1	101.1 (3)
N4—Sr3—Sr2^{ii}	48.48 (6)	N2—C5—Sr3^{vii}	104.6 (3)
N3^{ii}—Sr3—Sr2^{ii}	49.73 (9)	N1—C5—Sr3^{vii}	76.9 (2)
N3^{i}—Sr3—Sr2^{ii}	97.93 (8)	Sr1—C5—Sr3^{vii}	140.38 (6)
N1^{i}—Sr3—Sr2^{ii}	144.92 (8)	N2—C5—Sr3^{viii}	104.6 (3)
N1^{ii}—Sr3—Sr2^{ii}	97.70 (7)	N1—C5—Sr3^{viii}	76.9 (2)
C5^{i}—Sr3—Sr2^{ii}	168.16 (9)	Sr1—C5—Sr3^{viii}	140.38 (6)
C5^{ii}—Sr3—Sr2^{ii}	107.47 (6)	Sr3^{vii}—C5—Sr3^{viii}	78.50 (12)
Sr1—Sr3—Sr2^{ii}	66.676 (11)		

Symmetry codes: (i) −*x*+1/2, −*y*+1, *z*+1/2; (ii) −*x*+1/2, −*y*, *z*+1/2; (iii) −*x*, −*y*, −*z*+1; (iv) −*x*, −*y*+1, −*z*+1; (v) *x*, *y*+1, *z*; (vi) *x*, *y*−1, *z*; (vii) −*x*+1/2, −*y*, *z*−1/2; (viii) −*x*+1/2, −*y*+1, *z*−1/2; (ix) *x*−1/2, *y*, −*z*+1/2; (x) −*x*, −*y*, −*z*; (xi) −*x*+1, −*y*+1, −*z*+1; (xii) −*x*+1, −*y*, −*z*+1; (xiii) *x*+1/2, *y*, −*z*+1/2.