

Sr₁₁InSb₉ grown from molten In

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 Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{b-Sb}) = 0.001$ Å; R factor = 0.022; wR factor = 0.034; data-to-parameter ratio = 31.6.

Single crystals of the title compound, undecastrontium indium nonaantimonide, have been synthesized from a high-temperature reaction using a stoichiometric ratio of the elements Sr and Sb and excess In to act as a self-flux. The noncentrosymmetric structure has been determined from single-crystal X-ray diffraction data and has been found to be of the Ca₁₁InSb₉ structure type (Pearson code *oI84*). The structure can be visualized as being built of 11 Sr²⁺ cations, an [InSb₄]⁹⁻ tetrahedron, an [Sb₂]⁴⁻ dimer and three Sb³⁻ anions. One of six crystallographically independent Sr atoms, one of five Sb atoms and the In atom are located on positions with $\bar{2}$ symmetry.

Related literature

Sr₁₁InSb₉ is a Zintl (1939) compound and crystallizes in the Ca₁₁InSb₉ structure type (Cordier *et al.*, 1985*a*). The latter compound is reported to be a semiconductor with a large band gap (Young & Kauzlarich, 1995). The title compound is isotypic with Yb₁₁GaSb₉ (Bobev *et al.*, 2005), Yb₁₁InSb₉ and Eu₁₁GaSb₉ (Xia *et al.*, 2007), all with Pearson code *oI84* (Villars & Calvert, 1991). The relationship between the Ca₁₁InSb₉ structure type and that of Ca₂₁Mn₄Bi₁₈ has been discussed by Xia & Bobev (2007). Ionic radii were taken from Shannon (1976). Crystals of Sr₅In₂Sb₆ (Cordier *et al.*, 1985*b*) were also present in the reaction mixture.

Experimental

Crystal data

Sr ₁₁ InSb ₉	$V = 2839.6$ (5) Å ³
$M_r = 2174.39$	$Z = 4$
Orthorhombic, <i>Iba</i> 2	Mo $K\alpha$ radiation
$a = 12.3885$ (13) Å	$\mu = 29.64$ mm ⁻¹
$b = 13.1003$ (14) Å	$T = 120$ (2) K
$c = 17.4966$ (18) Å	$0.08 \times 0.05 \times 0.04$ mm

Data collection

Bruker SMART APEX diffractometer	Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
	$T_{\min} = 0.172$, $T_{\max} = 0.308$

 15129 measured reflections
 3124 independent reflections

 2972 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.046$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.034$
 $S = 0.90$
 3124 reflections
 99 parameters
 1 restraint

 $\Delta\rho_{\text{max}} = 0.90$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.00$ e Å⁻³
 Absolute structure: Flack (1983),
 1496 Friedel pairs
 Flack parameter: 0.017 (6)

Table 1

Selected bond lengths (Å).

Sr1—Sb3	3.1806 (9)	Sr3—Sb1 ^{iv}	3.5237 (10)
Sr1—Sb4	3.2466 (10)	Sr3—Sb2 ⁱⁱ	3.5434 (9)
Sr1—Sb5 ⁱ	3.3742 (10)	Sr4—Sb2 ⁱⁱ	3.1924 (10)
Sr1—Sb3 ⁱⁱ	3.3932 (9)	Sr4—Sb1	3.3574 (10)
Sr1—Sb2 ⁱⁱⁱ	3.4589 (9)	Sr4—Sb5 ^v	3.4647 (10)
Sr1—Sb1 ^{iv}	3.5094 (10)	Sr4—Sb4	3.5726 (10)
Sr2—Sb2 ⁱⁱⁱ	3.2082 (10)	Sr4—Sb4 ^v	3.6246 (10)
Sr2—Sb1	3.3012 (10)	Sr5—Sb3 ^{vii}	3.2068 (11)
Sr2—Sb4	3.6040 (10)	Sr5—Sb5 ^{vii}	3.3398 (11)
Sr2—Sb4 ^v	3.6137 (10)	Sr5—In1 ^{viii}	3.5475 (9)
Sr2—Sb3 ^v	3.6170 (9)	Sr5—Sb1 ^{ix}	3.6506 (9)
Sr2—Sb3 ⁱⁱ	3.6409 (10)	Sr6—Sb3	3.1990 (5)
Sr3—Sb3 ^{vi}	3.2340 (10)	Sr6—Sb3 ^x	3.1990 (5)
Sr3—Sb4	3.2347 (10)	Sr6—Sb5 ^{xi}	3.4575 (9)
Sr3—Sb5 ⁱⁱ	3.4584 (9)	Sb1—In1 ^{xii}	2.9213 (7)
Sr3—Sb5	3.5131 (9)	Sb4—Sb4 ^v	2.8437 (9)

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

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2002); program(s) used to refine structure: SHELXTL; molecular graphics: XP in SHELXTL; software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2135).

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Comment

The flux method was successfully applied for the synthesis of Yb₁₁GaSb₉ (Bobev *et al.*, 2005), Yb₁₁InSb₉ and Eu₁₁GaSb₉ (Xia *et al.*, 2007). The electronic structure and the properties of Yb₁₁GaSb₉ (Bobev *et al.*, 2005) are shown to be consistent with the Zintl concept (Zintl, 1939) and confirm that this class of compounds are small band-gap semiconductors or poor metals, as Eu₁₁InSb₉ and Yb₁₁InSb₉ (Xia *et al.*, 2007), whereas the Ca-analogs are reported to be semiconductors with larger band-gaps (Young & Kauzlarich, 1995). The close structural relationship between the Ca₁₁InSb₉ structure type (Cordier *et al.*, 1985a) and that of the monoclinic Ca₂₁Mn₄Bi₁₈ structure has been discussed in an earlier publication (Xia and Bobev, 2007). In connection with these studies, we undertook a similar synthetic approach in the Sr—In—Sb system.

Sr₁₁InSb₉ is a new member of the orthorhombic Ca₁₁InSb₉ structure type (Pearson's code *o*/84; Villars & Calvert, 1991). Its structure is very complex and has 12 crystallographically unique sites in the asymmetric unit. Thus it is difficult to explain in terms of packing of spheres; however, it can be rationalized simply using the Zintl formalism (Zintl, 1939). According to these rules and assuming a complete valence electron transfer from the less electronegative element, Sr, to the more electronegative In and Sb, one can visualize the structure as being built of eleven Sr²⁺ cations, an [InSb₄]⁹⁻ tetrahedron, an [Sb₂]⁴⁻ dimer, and three Sb³⁻ anions (Fig. 1).

The In—Sb bonding in the In centered tetrahedron has a covalent character with In—Sb distances ranging between 2.9213 (7) and 2.9312 (6) Å. These values are comparable to the In—Sb distances in the isotypic and isoelectronic Eu₁₁InSb₉, 2.913 (2) and 2.932 (2) Å (Xia *et al.*, 2007). We note that since Eu is divalent in Eu₁₁InSb₉ and since the ionic radii of Sr²⁺ and Eu²⁺ are nearly the same (Shannon, 1976), such comparison is straightforward. Not surprisingly, the Sb—Sb distance in Sr₁₁InSb₉ (2.8437 (9) Å) matches closely the Sb—Sb distance in the Eu analog (2.823 (2) Å) and also signifies strong covalent bonding. The interactions between the Sr²⁺ cations and the anions are more electrostatic in nature as evidenced by the larger coordination numbers and distances.

Experimental

Handling of the raw materials and the reaction products was done inside an Ar filled glove box. The reaction was carried out by loading the elements in an alumina crucible: Sr (Aldrich, pieces, distilled 99.99%), In (Alfa, shot, 99.99%), and Sb (Alfa, shot, 99.99%) in a ratio of 11:75:9. The large excess of In was intended as a metal flux. The crucible with the reaction mixture was then flame sealed under vacuum in a silica ampoule which was then placed in a furnace and heated to 1273 K at a rate of 300 K/h. The reaction proceeded at this temperature for 24 h before being cooled to 873 K at a rate of 10 K/h. At 873 K the ampoule was removed and the In flux was decanted. The main product of the reaction consisted of black crystals with irregular shapes, which were later determined to be the title compound. Also present were silver-metallic crystals with needle-like habit, which were found to be Sr₅In₂Sb₆ (Cordier *et al.*, 1985b). Note that Sr₁₁InSb₉ crystals decompose in air.

Refinement

The full occupancies for all sites were verified by freeing the site occupation factor for an individual atom, while other remaining parameters were kept fixed. This proved that all positions are fully occupied with corresponding deviations from full occupancy within 3σ . The maximum peak and deepest hole are located 1.36 Å away from Sr6 and 0.73 Å away from Sb4, respectively.

Figures

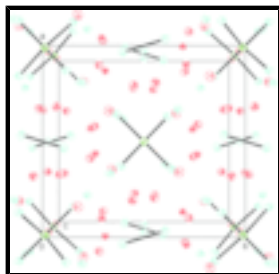


Fig. 1. A view of the structure of $\text{Sr}_{11}\text{InSb}_9$ along the c axis. Thermal ellipsoids are drawn at the 90% probability level. The Sr, In and Sb atoms are represented in red, green and light blue color, respectively.

undecastrontium indium nonaantimonide

Crystal data

$\text{Sr}_{11}\text{InSb}_9$

$M_r = 2174.39$

Orthorhombic, $Iba2$

Hall symbol: I 2 -2c

$a = 12.3885$ (13) Å

$b = 13.1003$ (14) Å

$c = 17.4966$ (18) Å

$V = 2839.6$ (5) Å³

$Z = 4$

$F_{000} = 3704$

$D_x = 5.086$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3124 reflections

$\theta = 2.3$ – 27.1°

$\mu = 29.64$ mm⁻¹

$T = 120$ (2) K

Irregular, black

$0.08 \times 0.05 \times 0.04$ mm

Data collection

Bruker SMART APEX
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 120$ (2) K

ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2003)

$T_{\min} = 0.172$, $T_{\max} = 0.308$

15129 measured reflections

3124 independent reflections

2972 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\text{max}} = 27.1^\circ$

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

$h = -15 \rightarrow 15$

$k = -16 \rightarrow 16$

$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.001P)^2]$
Least-squares matrix: full	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.022$	$(\Delta/\sigma)_{\max} < 0.001$
$wR(F^2) = 0.034$	$\Delta\rho_{\max} = 0.90 \text{ e } \text{\AA}^{-3}$
$S = 0.90$	$\Delta\rho_{\min} = -1.00 \text{ e } \text{\AA}^{-3}$
3124 reflections	Extinction correction: SHELXTL (Bruker, 2002)
99 parameters	Extinction coefficient: 0.000020 (3)
1 restraint	Absolute structure: Flack (1983), 1496 Friedel pairs
	Flack parameter: 0.017 (6)

Special details

Experimental. Crystals were selected in the glove box and cut in a Paratone N oil bath to the desired dimensions. A suitable crystal was then chosen mounted on the tip of a glass fiber and quickly placed under the cold nitrogen stream (*ca* 150 K) in a Bruker *SMART* CCD-based diffractometer.

Data collection is performed with four batch runs at $\varphi = 0.00^\circ$ (450 frames), at $\varphi = 90.00^\circ$ (450 frames), at $\varphi = 180.00^\circ$ (450 frames), and at $\varphi = 270.00^\circ$ (450 frames). Frame width = 0.40° in ω . Data are merged, corrected for decay, and treated with multi-scan absorption corrections.

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 $F^2 > 2\sigma(F^2)$ 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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	0.42681 (6)	0.22217 (5)	0.65758 (5)	0.01021 (16)
Sr2	0.68413 (6)	0.05401 (6)	0.62855 (4)	0.01204 (16)
Sr3	0.41024 (6)	0.22651 (6)	0.34159 (4)	0.01095 (17)
Sr4	0.68627 (7)	0.05890 (6)	0.36909 (5)	0.01248 (17)
Sr5	0.84036 (5)	0.17355 (5)	0.99994 (6)	0.01271 (14)
Sr6	0.0000	0.0000	0.67821 (6)	0.0126 (2)
Sb1	0.87132 (3)	0.11611 (3)	0.50258 (4)	0.01040 (10)
Sb2	0.0000	0.5000	0.25098 (5)	0.00951 (14)
Sb3	0.17692 (4)	0.17776 (4)	0.68278 (3)	0.01071 (11)
Sb4	0.46656 (4)	0.10383 (3)	0.49699 (3)	0.01059 (10)
Sb5	0.14600 (4)	0.13808 (4)	0.31116 (3)	0.01019 (11)
In1	0.0000	0.0000	0.39295 (4)	0.01094 (17)

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Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0093 (4)	0.0111 (4)	0.0103 (4)	-0.0002 (3)	0.0005 (3)	-0.0007 (3)
Sr2	0.0110 (4)	0.0122 (4)	0.0129 (4)	-0.0004 (3)	0.0026 (3)	0.0013 (3)
Sr3	0.0109 (4)	0.0118 (4)	0.0101 (4)	0.0007 (3)	-0.0004 (3)	0.0005 (3)
Sr4	0.0110 (4)	0.0133 (4)	0.0132 (4)	0.0009 (3)	-0.0022 (3)	-0.0020 (3)
Sr5	0.0142 (3)	0.0144 (4)	0.0095 (3)	0.0010 (3)	0.0000 (3)	-0.0006 (4)
Sr6	0.0100 (5)	0.0099 (5)	0.0179 (6)	-0.0008 (4)	0.000	0.000
Sb1	0.0097 (2)	0.0122 (2)	0.0092 (2)	-0.00036 (18)	-0.0001 (3)	-0.0003 (2)
Sb2	0.0094 (3)	0.0108 (3)	0.0084 (3)	0.0000 (4)	0.000	0.000
Sb3	0.0096 (2)	0.0123 (2)	0.0102 (3)	-0.0004 (2)	0.0004 (2)	-0.0011 (2)
Sb4	0.0119 (2)	0.0109 (2)	0.0089 (2)	0.00097 (18)	-0.0004 (3)	0.0003 (2)
Sb5	0.0093 (2)	0.0121 (2)	0.0091 (3)	0.0006 (2)	-0.0005 (2)	0.0004 (2)
In1	0.0103 (4)	0.0116 (4)	0.0109 (4)	-0.0009 (3)	0.000	0.000

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

Sr1—Sb3	3.1806 (9)	Sr5—Sr1 ^{xiv}	4.2183 (12)
Sr1—Sb4	3.2466 (10)	Sr6—Sb3	3.1990 (5)
Sr1—Sb5 ⁱ	3.3742 (10)	Sr6—Sb3 ^{xvi}	3.1990 (5)
Sr1—Sb3 ⁱⁱ	3.3932 (9)	Sr6—Sb5 ^{xvii}	3.4575 (9)
Sr1—Sb2 ⁱⁱⁱ	3.4589 (9)	Sr6—Sb5 ^{xv}	3.4575 (9)
Sr1—Sb1 ^{iv}	3.5094 (10)	Sr6—In1 ^{xv}	3.7572 (14)
Sr1—Sr6 ⁱⁱ	3.7682 (8)	Sr6—Sr1 ^{xviii}	3.7682 (8)
Sr1—Sr3 ^v	3.8005 (10)	Sr6—Sr1 ^{iv}	3.7682 (8)
Sr1—Sr2 ^{vi}	3.9034 (11)	Sr6—Sb1 ^{xix}	3.7814 (11)
Sr1—Sr2	3.9081 (11)	Sr6—Sb1 ^{vi}	3.7814 (11)
Sr1—Sr5 ^{vii}	4.2183 (11)	Sr6—Sr2 ^{xix}	4.0704 (9)
Sr1—Sr2 ^{iv}	4.2301 (11)	Sr6—Sr2 ^{vi}	4.0704 (9)
Sr2—Sb2 ⁱⁱⁱ	3.2082 (10)	Sr6—Sr5 ^{xx}	4.3371 (12)
Sr2—Sb1	3.3012 (10)	Sb1—In1 ^{viii}	2.9213 (7)
Sr2—Sb4	3.6040 (10)	Sb1—Sr1 ⁱⁱ	3.5094 (10)
Sr2—Sb4 ^{vi}	3.6137 (10)	Sb1—Sr3 ⁱⁱ	3.5238 (10)
Sr2—Sb3 ^{vi}	3.6170 (9)	Sb1—Sr5 ^{xxi}	3.6506 (9)
Sr2—Sb3 ⁱⁱ	3.6409 (10)	Sb1—Sr6 ^{viii}	3.7813 (11)
Sr2—Sr1 ^{vi}	3.9034 (11)	Sb1—Sr5 ^{vii}	3.8041 (9)
Sr2—Sb5 ^v	3.9812 (10)	Sb1—Sr5 ^{ix}	3.8143 (9)
Sr2—Sr6 ^{viii}	4.0704 (9)	Sb2—Sr4 ^{iv}	3.1924 (10)
Sr2—Sr5 ^{ix}	4.2067 (12)	Sb2—Sr4 ^{xxii}	3.1924 (10)
Sr2—Sr1 ⁱⁱ	4.2301 (11)	Sb2—Sr2 ^x	3.2081 (10)
Sr3—Sb3 ^x	3.2340 (10)	Sb2—Sr2 ^{xxiii}	3.2081 (10)
Sr3—Sb4	3.2347 (10)	Sb2—Sr1 ^x	3.4588 (9)

Sr3—Sb5 ⁱⁱ	3.4584 (9)	Sb2—Sr1 ^{xxiii}	3.4588 (9)
Sr3—Sb5	3.5131 (9)	Sb2—Sr3 ^{xxii}	3.5434 (9)
Sr3—Sb1 ^{iv}	3.5237 (10)	Sb2—Sr3 ^{iv}	3.5434 (9)
Sr3—Sb2 ⁱⁱ	3.5434 (9)	Sb3—Sr5 ^{xi}	3.2068 (11)
Sr3—Sr1 ^{xi}	3.8006 (10)	Sb3—Sr3 ⁱ	3.2340 (10)
Sr3—In1 ⁱⁱ	3.8575 (8)	Sb3—Sr1 ^{iv}	3.3932 (9)
Sr3—Sr4 ^{vi}	3.9550 (11)	Sb3—Sr2 ^{vi}	3.6170 (9)
Sr3—Sr4 ^{iv}	3.9790 (11)	Sb3—Sr2 ^{iv}	3.6408 (10)
Sr3—Sr4	4.0923 (11)	Sb3—Sr4 ^v	3.9903 (10)
Sr3—Sr5 ^{xi}	4.2184 (12)	Sb4—Sb4 ^{vi}	2.8437 (9)
Sr4—Sb2 ⁱⁱ	3.1924 (10)	Sb4—Sr2 ^{vi}	3.6137 (10)
Sr4—Sb1	3.3574 (10)	Sb4—Sr4 ^{vi}	3.6246 (10)
Sr4—Sb5 ^{vi}	3.4647 (10)	Sb4—Sr5 ^{vii}	3.7722 (9)
Sr4—Sb4	3.5726 (10)	Sb4—Sr5 ^{xi}	3.9107 (9)
Sr4—Sb4 ^{vi}	3.6246 (10)	Sb5—In1	2.9311 (6)
Sr4—Sr3 ^{vi}	3.9550 (11)	Sb5—Sr5 ^{xi}	3.3398 (11)
Sr4—Sr3 ⁱⁱ	3.9789 (11)	Sb5—Sr1 ^x	3.3743 (10)
Sr4—In1 ^{viii}	3.9844 (9)	Sb5—Sr6 ^{ix}	3.4575 (9)
Sr4—Sb3 ^{xi}	3.9903 (10)	Sb5—Sr3 ^{iv}	3.4584 (9)
Sr4—Sr5 ^{vii}	4.1993 (12)	Sb5—Sr4 ^{vi}	3.4647 (10)
Sr4—Sr5 ^{ix}	4.2613 (11)	Sb5—Sr2 ^{xi}	3.9812 (10)
Sr5—Sb3 ^v	3.2068 (11)	In1—Sb1 ^{vi}	2.9213 (7)
Sr5—Sb5 ^v	3.3398 (11)	In1—Sb1 ^{xix}	2.9213 (7)
Sr5—In1 ^{xii}	3.5475 (9)	In1—Sb5 ^{xvi}	2.9312 (6)
Sr5—Sb1 ^{xiii}	3.6506 (9)	In1—Sr5 ^{xi}	3.5475 (9)
Sr5—Sb4 ^{xiv}	3.7722 (9)	In1—Sr5 ^{xx}	3.5475 (9)
Sr5—Sb1 ^{xiv}	3.8041 (9)	In1—Sr6 ^{ix}	3.7572 (14)
Sr5—Sb1 ^{xv}	3.8143 (9)	In1—Sr3 ^{xviii}	3.8575 (8)
Sr5—Sb4 ^v	3.9108 (9)	In1—Sr3 ^{iv}	3.8575 (8)
Sr5—Sr4 ^{xiv}	4.1993 (12)	In1—Sr4 ^{xix}	3.9844 (9)
Sr5—Sr2 ^{xv}	4.2067 (12)	In1—Sr4 ^{vi}	3.9844 (9)
Sr5—Sr3 ^v	4.2185 (12)		
?...?	?		
Sb3—Sr1—Sb4	100.39 (2)	Sb4 ^{xiv} —Sr5—Sr2 ^{xv}	147.88 (3)
Sb3—Sr1—Sb5 ⁱ	74.26 (2)	Sb1 ^{xiv} —Sr5—Sr2 ^{xv}	100.93 (2)
Sb4—Sr1—Sb5 ⁱ	171.42 (3)	Sb1 ^{xv} —Sr5—Sr2 ^{xv}	48.302 (17)
Sb3—Sr1—Sb3 ⁱⁱ	160.29 (3)	Sb4 ^v —Sr5—Sr2 ^{xv}	52.715 (16)
Sb4—Sr1—Sb3 ⁱⁱ	99.12 (2)	Sr4 ^{xiv} —Sr5—Sr2 ^{xv}	147.88 (3)
Sb5 ⁱ —Sr1—Sb3 ⁱⁱ	86.04 (2)	Sb3 ^v —Sr5—Sr3 ^v	127.10 (2)
Sb3—Sr1—Sb2 ⁱⁱⁱ	92.05 (2)	Sb5 ^v —Sr5—Sr3 ^v	53.885 (19)

supplementary materials

Sb4—Sr1—Sb2 ⁱⁱⁱ	88.12 (2)	In1 ^{xii} —Sr5—Sr3 ^v	99.74 (3)
Sb5 ⁱ —Sr1—Sb2 ⁱⁱⁱ	98.65 (3)	Sb1 ^{xiii} —Sr5—Sr3 ^v	139.66 (3)
Sb3 ⁱⁱ —Sr1—Sb2 ⁱⁱⁱ	91.39 (2)	Sb4 ^{xiv} —Sr5—Sr3 ^v	109.30 (2)
Sb3—Sr1—Sb1 ^{iv}	91.54 (2)	Sb1 ^{xiv} —Sr5—Sr3 ^v	51.795 (17)
Sb4—Sr1—Sb1 ^{iv}	69.46 (2)	Sb1 ^{xv} —Sr5—Sr3 ^v	104.22 (2)
Sb5 ⁱ —Sr1—Sb1 ^{iv}	103.62 (2)	Sb4 ^v —Sr5—Sr3 ^v	46.706 (17)
Sb3 ⁱⁱ —Sr1—Sb1 ^{iv}	92.64 (2)	Sr4 ^{xiv} —Sr5—Sr3 ^v	56.416 (19)
Sb2 ⁱⁱⁱ —Sr1—Sb1 ^{iv}	157.58 (3)	Sr2 ^{xv} —Sr5—Sr3 ^v	97.43 (2)
Sb3—Sr1—Sr6 ⁱⁱ	113.43 (2)	Sb3 ^v —Sr5—Sr1 ^{xiv}	52.249 (19)
Sb4—Sr1—Sr6 ⁱⁱ	120.51 (3)	Sb5 ^v —Sr5—Sr1 ^{xiv}	131.08 (2)
Sb5 ⁱ —Sr1—Sr6 ⁱⁱ	57.59 (2)	In1 ^{xii} —Sr5—Sr1 ^{xiv}	99.87 (2)
Sb3 ⁱⁱ —Sr1—Sr6 ⁱⁱ	52.747 (13)	Sb1 ^{xiii} —Sr5—Sr1 ^{xiv}	52.369 (18)
Sb2 ⁱⁱⁱ —Sr1—Sr6 ⁱⁱ	134.78 (3)	Sb4 ^{xiv} —Sr5—Sr1 ^{xiv}	47.542 (16)
Sb1 ^{iv} —Sr1—Sr6 ⁱⁱ	62.49 (2)	Sb1 ^{xiv} —Sr5—Sr1 ^{xiv}	103.23 (2)
Sb3—Sr1—Sr3 ^v	113.72 (2)	Sb1 ^{xv} —Sr5—Sr1 ^{xiv}	104.21 (2)
Sb4—Sr1—Sr3 ^v	131.28 (3)	Sb4 ^v —Sr5—Sr1 ^{xiv}	138.51 (3)
Sb5 ⁱ —Sr1—Sr3 ^v	57.265 (19)	Sr4 ^{xiv} —Sr5—Sr1 ^{xiv}	98.04 (2)
Sb3 ⁱⁱ —Sr1—Sr3 ^v	53.062 (19)	Sr2 ^{xv} —Sr5—Sr1 ^{xiv}	101.21 (3)
Sb2 ⁱⁱⁱ —Sr1—Sr3 ^v	58.21 (2)	Sr3 ^v —Sr5—Sr1 ^{xiv}	151.57 (2)
Sb1 ^{iv} —Sr1—Sr3 ^v	138.56 (3)	Sb3—Sr6—Sb3 ^{xvi}	177.13 (4)
Sr6 ⁱⁱ —Sr1—Sr3 ^v	77.09 (2)	Sb3—Sr6—Sb5 ^{xvii}	87.749 (19)
Sb3—Sr1—Sr2 ^{vi}	60.385 (19)	Sb3 ^{xvi} —Sr6—Sb5 ^{xvii}	90.321 (19)
Sb4—Sr1—Sr2 ^{vi}	59.880 (19)	Sb3—Sr6—Sb5 ^{xv}	90.322 (19)
Sb5 ⁱ —Sr1—Sr2 ^{vi}	120.82 (3)	Sb3 ^{xvi} —Sr6—Sb5 ^{xv}	87.749 (19)
Sb3 ⁱⁱ —Sr1—Sr2 ^{vi}	134.15 (3)	Sb5 ^{xvii} —Sr6—Sb5 ^{xv}	95.44 (3)
Sb2 ⁱⁱⁱ —Sr1—Sr2 ^{vi}	51.232 (18)	Sb3—Sr6—In1 ^{xv}	88.57 (2)
Sb1 ^{iv} —Sr1—Sr2 ^{vi}	112.96 (3)	Sb3 ^{xvi} —Sr6—In1 ^{xv}	88.57 (2)
Sr6 ⁱⁱ —Sr1—Sr2 ^{vi}	172.95 (3)	Sb5 ^{xvii} —Sr6—In1 ^{xv}	47.719 (16)
Sr3 ^v —Sr1—Sr2 ^{vi}	108.13 (3)	Sb5 ^{xv} —Sr6—In1 ^{xv}	47.719 (16)
Sb3—Sr1—Sr2	135.14 (3)	Sb3—Sr6—Sr1 ^{xviii}	122.728 (16)
Sb4—Sr1—Sr2	59.643 (19)	Sb3 ^{xvi} —Sr6—Sr1 ^{xviii}	57.598 (16)
Sb5 ⁱ —Sr1—Sr2	128.86 (3)	Sb5 ^{xvii} —Sr6—Sr1 ^{xviii}	134.08 (3)
Sb3 ⁱⁱ —Sr1—Sr2	59.32 (2)	Sb5 ^{xv} —Sr6—Sr1 ^{xviii}	55.475 (16)
Sb2 ⁱⁱⁱ —Sr1—Sr2	51.188 (17)	In1 ^{xv} —Sr6—Sr1 ^{xviii}	95.50 (2)
Sb1 ^{iv} —Sr1—Sr2	113.55 (3)	Sb3—Sr6—Sr1 ^{iv}	57.598 (16)
Sr6 ⁱⁱ —Sr1—Sr2	111.14 (2)	Sb3 ^{xvi} —Sr6—Sr1 ^{iv}	122.728 (16)
Sr3 ^v —Sr1—Sr2	71.65 (2)	Sb5 ^{xvii} —Sr6—Sr1 ^{iv}	55.475 (16)
Sr2 ^{vi} —Sr1—Sr2	75.39 (2)	Sb5 ^{xv} —Sr6—Sr1 ^{iv}	134.08 (3)
Sb3—Sr1—Sr5 ^{vii}	144.63 (3)	In1 ^{xv} —Sr6—Sr1 ^{iv}	95.50 (2)
Sb4—Sr1—Sr5 ^{vii}	59.01 (2)	Sr1 ^{xviii} —Sr6—Sr1 ^{iv}	169.01 (4)
Sb5 ⁱ —Sr1—Sr5 ^{vii}	121.86 (2)	Sb3—Sr6—Sb1 ^{xix}	90.94 (2)

Sb3 ⁱⁱ —Sr1—Sr5 ^{vii}	48.352 (18)	Sb3 ^{xvi} —Sr6—Sb1 ^{xix}	91.39 (2)
Sb2 ⁱⁱⁱ —Sr1—Sr5 ^{vii}	113.71 (2)	Sb5 ^{xvii} —Sr6—Sb1 ^{xix}	96.647 (14)
Sb1 ^{iv} —Sr1—Sr5 ^{vii}	55.470 (17)	Sb5 ^{xv} —Sr6—Sb1 ^{xix}	167.89 (3)
Sr6 ⁱⁱ —Sr1—Sr5 ^{vii}	65.50 (2)	In1 ^{xv} —Sr6—Sb1 ^{xix}	144.359 (13)
Sr3 ^v —Sr1—Sr5 ^{vii}	100.71 (2)	Sr1 ^{xviii} —Sr6—Sb1 ^{xix}	114.34 (3)
Sr2 ^{vi} —Sr1—Sr5 ^{vii}	117.12 (2)	Sr1 ^{iv} —Sr6—Sb1 ^{xix}	55.401 (16)
Sr2—Sr1—Sr5 ^{vii}	62.599 (19)	Sb3—Sr6—Sb1 ^{vi}	91.39 (2)
Sb3—Sr1—Sr2 ^{iv}	56.749 (18)	Sb3 ^{xvi} —Sr6—Sb1 ^{vi}	90.94 (2)
Sb4—Sr1—Sr2 ^{iv}	109.57 (2)	Sb5 ^{xvii} —Sr6—Sb1 ^{vi}	167.89 (3)
Sb5 ⁱ —Sr1—Sr2 ^{iv}	61.937 (18)	Sb5 ^{xv} —Sr6—Sb1 ^{vi}	96.647 (14)
Sb3 ⁱⁱ —Sr1—Sr2 ^{iv}	113.38 (2)	In1 ^{xv} —Sr6—Sb1 ^{vi}	144.359 (13)
Sb2 ⁱⁱⁱ —Sr1—Sr2 ^{iv}	145.72 (3)	Sr1 ^{xviii} —Sr6—Sb1 ^{vi}	55.401 (16)
Sb1 ^{iv} —Sr1—Sr2 ^{iv}	49.425 (17)	Sr1 ^{iv} —Sr6—Sb1 ^{vi}	114.34 (3)
Sr6 ⁱⁱ —Sr1—Sr2 ^{iv}	60.858 (17)	Sb1 ^{xix} —Sr6—Sb1 ^{vi}	71.28 (3)
Sr3 ^v —Sr1—Sr2 ^{iv}	117.96 (2)	Sb3—Sr6—Sr2 ^{xix}	122.512 (16)
Sr2 ^{vi} —Sr1—Sr2 ^{iv}	112.12 (2)	Sb3 ^{xvi} —Sr6—Sr2 ^{xix}	58.210 (15)
Sr2—Sr1—Sr2 ^{iv}	162.72 (3)	Sb5 ^{xvii} —Sr6—Sr2 ^{xix}	63.240 (15)
Sr5 ^{vii} —Sr1—Sr2 ^{iv}	100.55 (2)	Sb5 ^{xv} —Sr6—Sr2 ^{xix}	137.52 (2)
Sb2 ⁱⁱⁱ —Sr2—Sb1	178.44 (3)	In1 ^{xv} —Sr6—Sr2 ^{xix}	102.325 (18)
Sb2 ⁱⁱⁱ —Sr2—Sb4	86.25 (2)	Sr1 ^{xviii} —Sr6—Sr2 ^{xix}	112.258 (18)
Sb1—Sr2—Sb4	93.11 (2)	Sr1 ^{iv} —Sr6—Sr2 ^{xix}	65.186 (16)
Sb2 ⁱⁱⁱ —Sr2—Sb4 ^{vi}	86.09 (2)	Sb1 ^{xix} —Sr6—Sr2 ^{xix}	49.557 (15)
Sb1—Sr2—Sb4 ^{vi}	94.51 (2)	Sb1 ^{vi} —Sr6—Sr2 ^{xix}	107.56 (3)
Sb4—Sr2—Sb4 ^{vi}	46.406 (18)	Sb3—Sr6—Sr2 ^{vi}	58.210 (15)
Sb2 ⁱⁱⁱ —Sr2—Sb3 ^{vi}	88.74 (2)	Sb3 ^{xvi} —Sr6—Sr2 ^{vi}	122.513 (16)
Sb1—Sr2—Sb3 ^{vi}	92.74 (2)	Sb5 ^{xvii} —Sr6—Sr2 ^{vi}	137.52 (2)
Sb4—Sr2—Sb3 ^{vi}	132.49 (3)	Sb5 ^{xv} —Sr6—Sr2 ^{vi}	63.240 (15)
Sb4 ^{vi} —Sr2—Sb3 ^{vi}	86.14 (2)	In1 ^{xv} —Sr6—Sr2 ^{vi}	102.325 (19)
Sb2 ⁱⁱⁱ —Sr2—Sb3 ⁱⁱ	91.23 (2)	Sr1 ^{xviii} —Sr6—Sr2 ^{vi}	65.186 (16)
Sb1—Sr2—Sb3 ⁱⁱ	87.33 (2)	Sr1 ^{iv} —Sr6—Sr2 ^{vi}	112.258 (18)
Sb4—Sr2—Sb3 ⁱⁱ	88.47 (2)	Sb1 ^{xix} —Sr6—Sr2 ^{vi}	107.56 (3)
Sb4 ^{vi} —Sr2—Sb3 ⁱⁱ	134.88 (3)	Sb1 ^{vi} —Sr6—Sr2 ^{vi}	49.557 (15)
Sb3 ^{vi} —Sr2—Sb3 ⁱⁱ	138.89 (3)	Sr2 ^{xix} —Sr6—Sr2 ^{vi}	155.35 (4)
Sb2 ⁱⁱⁱ —Sr2—Sr1 ^{vi}	57.205 (18)	Sb3—Sr6—Sr5 ^{xx}	135.40 (3)
Sb1—Sr2—Sr1 ^{vi}	124.24 (3)	Sb3 ^{xvi} —Sr6—Sr5 ^{xx}	47.463 (18)
Sb4—Sr2—Sr1 ^{vi}	89.29 (2)	Sb5 ^{xvii} —Sr6—Sr5 ^{xx}	121.303 (14)
Sb4 ^{vi} —Sr2—Sr1 ^{vi}	50.998 (18)	Sb5 ^{xv} —Sr6—Sr5 ^{xx}	116.624 (14)
Sb3 ^{vi} —Sr2—Sr1 ^{vi}	49.860 (18)	In1 ^{xv} —Sr6—Sr5 ^{xx}	135.988 (15)
Sb3 ⁱⁱ —Sr2—Sr1 ^{vi}	148.43 (3)	Sr1 ^{xviii} —Sr6—Sr5 ^{xx}	62.257 (18)
Sb2 ⁱⁱⁱ —Sr2—Sr1	57.150 (18)	Sr1 ^{iv} —Sr6—Sr5 ^{xx}	109.13 (2)
Sb1—Sr2—Sr1	121.39 (3)	Sb1 ^{xix} —Sr6—Sr5 ^{xx}	55.539 (18)

supplementary materials

Sb4—Sr2—Sr1	51.015 (19)	Sb1 ^{vi} —Sr6—Sr5 ^{xx}	52.908 (17)
Sb4 ^{vi} —Sr2—Sr1	89.08 (2)	Sr2 ^{xxix} —Sr6—Sr5 ^{xx}	59.948 (17)
Sb3 ^{vi} —Sr2—Sr1	145.82 (3)	Sr2 ^{vi} —Sr6—Sr5 ^{xx}	101.17 (2)
Sb3 ⁱⁱ —Sr2—Sr1	53.280 (18)	In1 ^{viii} —Sb1—Sr2	133.90 (2)
Sr1 ^{vi} —Sr2—Sr1	102.61 (2)	In1 ^{viii} —Sb1—Sr4	78.44 (2)
Sb2 ⁱⁱⁱ —Sr2—Sb5 ^v	84.32 (2)	Sr2—Sb1—Sr4	85.97 (2)
Sb1—Sr2—Sb5 ^v	95.53 (2)	In1 ^{viii} —Sb1—Sr1 ⁱⁱ	135.63 (2)
Sb4—Sr2—Sb5 ^v	149.07 (3)	Sr2—Sb1—Sr1 ⁱⁱ	76.73 (2)
Sb4 ^{vi} —Sr2—Sb5 ^v	160.48 (3)	Sr4—Sb1—Sr1 ⁱⁱ	143.72 (2)
Sb3 ^{vi} —Sr2—Sb5 ^v	76.71 (2)	In1 ^{viii} —Sb1—Sr3 ⁱⁱ	72.85 (2)
Sb3 ⁱⁱ —Sr2—Sb5 ^v	62.406 (17)	Sr2—Sb1—Sr3 ⁱⁱ	140.72 (2)
Sr1 ^{vi} —Sr2—Sb5 ^v	109.76 (2)	Sr4—Sb1—Sr3 ⁱⁱ	70.61 (2)
Sr1—Sr2—Sb5 ^v	99.84 (2)	Sr1 ⁱⁱ —Sb1—Sr3 ⁱⁱ	103.75 (2)
Sb2 ⁱⁱⁱ —Sr2—Sr6 ^{viii}	120.18 (3)	In1 ^{viii} —Sb1—Sr5 ^{xxi}	64.221 (17)
Sb1—Sr2—Sr6 ^{viii}	60.66 (2)	Sr2—Sb1—Sr5 ^{xxi}	138.30 (3)
Sb4—Sr2—Sr6 ^{viii}	152.47 (3)	Sr4—Sb1—Sr5 ^{xxi}	134.85 (3)
Sb4 ^{vi} —Sr2—Sr6 ^{viii}	122.22 (2)	Sr1 ⁱⁱ —Sb1—Sr5 ^{xxi}	72.16 (2)
Sb3 ^{vi} —Sr2—Sr6 ^{viii}	48.743 (13)	Sr3 ⁱⁱ —Sb1—Sr5 ^{xxi}	74.66 (2)
Sb3 ⁱⁱ —Sr2—Sr6 ^{viii}	97.80 (2)	In1 ^{viii} —Sb1—Sr6 ^{viii}	95.40 (2)
Sr1 ^{vi} —Sr2—Sr6 ^{viii}	98.60 (2)	Sr2—Sb1—Sr6 ^{viii}	69.78 (2)
Sr1—Sr2—Sr6 ^{viii}	148.70 (3)	Sr4—Sb1—Sr6 ^{viii}	139.77 (2)
Sb5 ^v —Sr2—Sr6 ^{viii}	50.847 (18)	Sr1 ⁱⁱ —Sb1—Sr6 ^{viii}	62.111 (18)
Sb2 ⁱⁱⁱ —Sr2—Sr5 ^{ix}	121.87 (2)	Sr3 ⁱⁱ —Sb1—Sr6 ^{viii}	145.822 (19)
Sb1—Sr2—Sr5 ^{ix}	59.623 (19)	Sr5 ^{xxi} —Sb1—Sr6 ^{viii}	71.380 (18)
Sb4—Sr2—Sr5 ^{ix}	97.51 (2)	In1 ^{viii} —Sb1—Sr5 ^{vii}	138.19 (3)
Sb4 ^{vi} —Sr2—Sr5 ^{ix}	59.433 (18)	Sr2—Sb1—Sr5 ^{vii}	72.68 (2)
Sb3 ^{vi} —Sr2—Sr5 ^{ix}	47.663 (18)	Sr4—Sb1—Sr5 ^{vii}	71.49 (2)
Sb3 ⁱⁱ —Sr2—Sr5 ^{ix}	146.58 (3)	Sr1 ⁱⁱ —Sb1—Sr5 ^{vii}	72.97 (2)
Sr1 ^{vi} —Sr2—Sr5 ^{ix}	64.83 (2)	Sr3 ⁱⁱ —Sb1—Sr5 ^{vii}	70.17 (2)
Sr1—Sr2—Sr5 ^{ix}	147.59 (3)	Sr5 ^{xxi} —Sb1—Sr5 ^{vii}	121.670 (15)
Sb5 ^v —Sr2—Sr5 ^{ix}	112.47 (2)	Sr6 ^{viii} —Sb1—Sr5 ^{vii}	126.29 (3)
Sr6 ^{viii} —Sr2—Sr5 ^{ix}	63.174 (19)	In1 ^{viii} —Sb1—Sr5 ^{ix}	61.896 (17)
Sb2 ⁱⁱⁱ —Sr2—Sr1 ⁱⁱ	125.31 (3)	Sr2—Sb1—Sr5 ^{ix}	72.08 (2)
Sb1—Sr2—Sr1 ⁱⁱ	53.848 (19)	Sr4—Sb1—Sr5 ^{ix}	72.59 (2)
Sb4—Sr2—Sr1 ⁱⁱ	118.86 (2)	Sr1 ⁱⁱ —Sb1—Sr5 ^{ix}	129.02 (3)
Sb4 ^{vi} —Sr2—Sr1 ⁱⁱ	147.17 (3)	Sr3 ⁱⁱ —Sb1—Sr5 ^{ix}	125.88 (3)
Sb3 ^{vi} —Sr2—Sr1 ⁱⁱ	102.25 (2)	Sr5 ^{xxi} —Sb1—Sr5 ^{ix}	107.658 (16)
Sb3 ⁱⁱ —Sr2—Sr1 ⁱⁱ	46.933 (16)	Sr6 ^{viii} —Sb1—Sr5 ^{ix}	69.637 (17)
Sr1 ^{vi} —Sr2—Sr1 ⁱⁱ	151.29 (3)	Sr5 ^{vii} —Sb1—Sr5 ^{ix}	130.627 (14)
Sr1—Sr2—Sr1 ⁱⁱ	99.985 (19)	Sr4 ^{iv} —Sb2—Sr4 ^{xxii}	99.32 (4)
Sb5 ^v —Sr2—Sr1 ⁱⁱ	48.409 (16)	Sr4 ^{iv} —Sb2—Sr2 ^x	153.237 (17)

Sr6 ^{viii} —Sr2—Sr1 ⁱⁱ	53.956 (15)	Sr4 ^{xxii} —Sb2—Sr2 ^x	88.370 (18)
Sr5 ^{ix} —Sr2—Sr1 ⁱⁱ	103.21 (2)	Sr4 ^{iv} —Sb2—Sr2 ^{xxiii}	88.370 (18)
Sb3 ^x —Sr3—Sb4	170.71 (3)	Sr4 ^{xxii} —Sb2—Sr2 ^{xxiii}	153.237 (17)
Sb3 ^x —Sr3—Sb5 ⁱⁱ	87.18 (2)	Sr2 ^x —Sb2—Sr2 ^{xxiii}	96.22 (4)
Sb4—Sr3—Sb5 ⁱⁱ	101.66 (2)	Sr4 ^{iv} —Sb2—Sr1 ^x	85.00 (2)
Sb3 ^x —Sr3—Sb5	71.732 (19)	Sr4 ^{xxii} —Sb2—Sr1 ^x	134.33 (2)
Sb4—Sr3—Sb5	99.47 (2)	Sr2 ^x —Sb2—Sr1 ^x	71.66 (2)
Sb5 ⁱⁱ —Sr3—Sb5	158.87 (3)	Sr2 ^{xxiii} —Sb2—Sr1 ^x	71.56 (2)
Sb3 ^x —Sr3—Sb1 ^{iv}	114.47 (3)	Sr4 ^{iv} —Sb2—Sr1 ^{xxiii}	134.33 (2)
Sb4—Sr3—Sb1 ^{iv}	69.41 (2)	Sr4 ^{xxii} —Sb2—Sr1 ^{xxiii}	85.00 (2)
Sb5 ⁱⁱ —Sr3—Sb1 ^{iv}	86.48 (2)	Sr2 ^x —Sb2—Sr1 ^{xxiii}	71.56 (2)
Sb5—Sr3—Sb1 ^{iv}	100.75 (2)	Sr2 ^{xxiii} —Sb2—Sr1 ^{xxiii}	71.66 (2)
Sb3 ^x —Sr3—Sb2 ⁱⁱ	92.58 (2)	Sr1 ^x —Sb2—Sr1 ^{xxiii}	123.61 (4)
Sb4—Sr3—Sb2 ⁱⁱ	83.82 (2)	Sr4 ^{iv} —Sb2—Sr3 ^{xxii}	71.70 (2)
Sb5 ⁱⁱ —Sr3—Sb2 ⁱⁱ	95.49 (2)	Sr4 ^{xxii} —Sb2—Sr3 ^{xxii}	74.62 (2)
Sb5—Sr3—Sb2 ⁱⁱ	87.044 (19)	Sr2 ^x —Sb2—Sr3 ^{xxii}	134.96 (2)
Sb1 ^{iv} —Sr3—Sb2 ⁱⁱ	152.95 (3)	Sr2 ^{xxiii} —Sb2—Sr3 ^{xxii}	83.74 (2)
Sb3 ^x —Sr3—Sr1 ^{xi}	56.998 (19)	Sr1 ^x —Sb2—Sr3 ^{xxii}	146.491 (17)
Sb4—Sr3—Sr1 ^{xi}	126.16 (3)	Sr1 ^{xxiii} —Sb2—Sr3 ^{xxii}	65.730 (16)
Sb5 ⁱⁱ —Sr3—Sr1 ^{xi}	55.156 (19)	Sr4 ^{iv} —Sb2—Sr3 ^{iv}	74.62 (2)
Sb5—Sr3—Sr1 ^{xi}	111.20 (2)	Sr4 ^{xxii} —Sb2—Sr3 ^{iv}	71.70 (2)
Sb1 ^{iv} —Sr3—Sr1 ^{xi}	139.34 (3)	Sr2 ^x —Sb2—Sr3 ^{iv}	83.74 (2)
Sb2 ⁱⁱ —Sr3—Sr1 ^{xi}	56.064 (19)	Sr2 ^{xxiii} —Sb2—Sr3 ^{iv}	134.96 (2)
Sb3 ^x —Sr3—In1 ⁱⁱ	86.35 (2)	Sr1 ^x —Sb2—Sr3 ^{iv}	65.730 (16)
Sb4—Sr3—In1 ⁱⁱ	101.74 (2)	Sr1 ^{xxiii} —Sb2—Sr3 ^{iv}	146.491 (16)
Sb5 ⁱⁱ —Sr3—In1 ⁱⁱ	46.846 (13)	Sr3 ^{xxii} —Sb2—Sr3 ^{iv}	126.84 (4)
Sb5—Sr3—In1 ⁱⁱ	127.60 (2)	Sr1—Sb3—Sr6	142.80 (2)
Sb1 ^{iv} —Sr3—In1 ⁱⁱ	46.356 (16)	Sr1—Sb3—Sr5 ^{xi}	85.97 (2)
Sb2 ⁱⁱ —Sr3—In1 ⁱⁱ	142.33 (2)	Sr6—Sb3—Sr5 ^{xi}	85.23 (3)
Sr1 ^{xi} —Sr3—In1 ⁱⁱ	93.33 (2)	Sr1—Sb3—Sr3 ⁱ	111.91 (3)
Sb3 ^x —Sr3—Sr4 ^{vi}	111.73 (3)	Sr6—Sb3—Sr3 ⁱ	94.30 (3)
Sb4—Sr3—Sr4 ^{vi}	59.55 (2)	Sr5 ^{xi} —Sb3—Sr3 ⁱ	147.30 (2)
Sb5 ⁱⁱ —Sr3—Sr4 ^{vi}	139.37 (3)	Sr1—Sb3—Sr1 ^{iv}	143.14 (2)
Sb5—Sr3—Sr4 ^{vi}	54.898 (18)	Sr6—Sb3—Sr1 ^{iv}	69.655 (18)
Sb1 ^{iv} —Sr3—Sr4 ^{vi}	114.49 (3)	Sr5 ^{xi} —Sb3—Sr1 ^{iv}	79.40 (2)
Sb2 ⁱⁱ —Sr3—Sr4 ^{vi}	50.027 (18)	Sr3 ⁱ —Sb3—Sr1 ^{iv}	69.94 (2)
Sr1 ^{xi} —Sr3—Sr4 ^{vi}	104.45 (3)	Sr1—Sb3—Sr2 ^{vi}	69.75 (2)
In1 ⁱⁱ —Sr3—Sr4 ^{vi}	159.54 (3)	Sr6—Sb3—Sr2 ^{vi}	73.047 (18)
Sb3 ^x —Sr3—Sr4 ^{iv}	66.24 (2)	Sr5 ^{xi} —Sb3—Sr2 ^{vi}	75.85 (2)
Sb4—Sr3—Sr4 ^{iv}	113.57 (3)	Sr3 ⁱ —Sb3—Sr2 ^{vi}	135.22 (2)
Sb5 ⁱⁱ —Sr3—Sr4 ^{iv}	104.19 (2)	Sr1 ^{iv} —Sb3—Sr2 ^{vi}	136.45 (2)

supplementary materials

Sb5—Sr3—Sr4 ^{iv}	66.52 (2)	Sr1—Sb3—Sr2 ^{iv}	76.32 (2)
Sb1 ^{iv} —Sr3—Sr4 ^{iv}	52.740 (17)	Sr6—Sb3—Sr2 ^{iv}	135.47 (2)
Sb2 ⁱⁱ —Sr3—Sr4 ^{iv}	149.83 (3)	Sr5 ^{xi} —Sb3—Sr2 ^{iv}	76.01 (2)
Sr1 ^{xi} —Sr3—Sr4 ^{iv}	118.91 (3)	Sr3 ⁱ —Sb3—Sr2 ^{iv}	81.83 (2)
In1 ⁱⁱ —Sr3—Sr4 ^{iv}	61.098 (17)	Sr1 ^{iv} —Sb3—Sr2 ^{iv}	67.40 (2)
Sr4 ^{vi} —Sr3—Sr4 ^{iv}	116.26 (2)	Sr2 ^{vi} —Sb3—Sr2 ^{iv}	136.90 (2)
Sb3 ^x —Sr3—Sr4	126.02 (3)	Sr1—Sb3—Sr4 ^v	76.78 (2)
Sb4—Sr3—Sr4	56.930 (19)	Sr6—Sb3—Sr4 ^v	91.57 (2)
Sb5 ⁱⁱ —Sr3—Sr4	65.64 (2)	Sr5 ^{xi} —Sb3—Sr4 ^v	146.78 (2)
Sb5—Sr3—Sr4	128.28 (3)	Sr3 ⁱ —Sb3—Sr4 ^v	65.87 (2)
Sb1 ^{iv} —Sr3—Sr4	109.53 (2)	Sr1 ^{iv} —Sb3—Sr4 ^v	130.15 (2)
Sb2 ⁱⁱ —Sr3—Sr4	48.779 (16)	Sr2 ^{vi} —Sb3—Sr4 ^v	71.615 (18)
Sr1 ^{xi} —Sr3—Sr4	69.37 (2)	Sr2 ^{iv} —Sb3—Sr4 ^v	125.39 (2)
In1 ⁱⁱ —Sr3—Sr4	103.30 (2)	Sb4 ^{vi} —Sb4—Sr3	122.558 (17)
Sr4 ^{vi} —Sr3—Sr4	74.40 (2)	Sb4 ^{vi} —Sb4—Sr1	120.068 (16)
Sr4 ^{iv} —Sr3—Sr4	161.36 (3)	Sr3—Sb4—Sr1	117.22 (2)
Sb3 ^x —Sr3—Sr5 ^{xi}	112.48 (2)	Sb4 ^{vi} —Sb4—Sr4	67.693 (18)
Sb4—Sr3—Sr5 ^{xi}	61.64 (2)	Sr3—Sb4—Sr4	73.72 (2)
Sb5 ⁱⁱ —Sr3—Sr5 ^{xi}	143.80 (3)	Sr1—Sb4—Sr4	137.42 (2)
Sb5—Sr3—Sr5 ^{xi}	50.174 (18)	Sb4 ^{vi} —Sb4—Sr2	66.976 (18)
Sb1 ^{iv} —Sr3—Sr5 ^{xi}	58.031 (18)	Sr3—Sb4—Sr2	142.01 (2)
Sb2 ⁱⁱ —Sr3—Sr5 ^{xi}	112.77 (2)	Sr1—Sb4—Sr2	69.34 (2)
Sr1 ^{xi} —Sr3—Sr5 ^{xi}	160.88 (3)	Sr4—Sb4—Sr2	78.488 (19)
In1 ⁱⁱ —Sr3—Sr5 ^{xi}	102.23 (2)	Sb4 ^{vi} —Sb4—Sr2 ^{vi}	66.620 (19)
Sr4 ^{vi} —Sr3—Sr5 ^{xi}	62.750 (19)	Sr3—Sb4—Sr2 ^{vi}	135.10 (2)
Sr4 ^{iv} —Sr3—Sr5 ^{xi}	61.549 (19)	Sr1—Sb4—Sr2 ^{vi}	69.12 (2)
Sr4—Sr3—Sr5 ^{xi}	116.71 (2)	Sr4—Sb4—Sr2 ^{vi}	134.29 (2)
Sb2 ⁱⁱ —Sr4—Sb1	176.25 (3)	Sr2—Sb4—Sr2 ^{vi}	82.87 (3)
Sb2 ⁱⁱ —Sr4—Sb5 ^{vi}	93.68 (2)	Sb4 ^{vi} —Sb4—Sr4 ^{vi}	65.767 (19)
Sb1—Sr4—Sb5 ^{vi}	87.72 (2)	Sr3—Sb4—Sr4 ^{vi}	70.16 (2)
Sb2 ⁱⁱ —Sr4—Sb4	83.95 (2)	Sr1—Sb4—Sr4 ^{vi}	137.39 (2)
Sb1—Sr4—Sb4	92.73 (2)	Sr4—Sb4—Sr4 ^{vi}	85.09 (3)
Sb5 ^{vi} —Sr4—Sb4	139.72 (3)	Sr2—Sb4—Sr4 ^{vi}	132.72 (2)
Sb2 ⁱⁱ —Sr4—Sb4 ^{vi}	83.10 (2)	Sr2 ^{vi} —Sb4—Sr4 ^{vi}	77.696 (18)
Sb1—Sr4—Sb4 ^{vi}	93.35 (2)	Sb4 ^{vi} —Sb4—Sr5 ^{vii}	123.70 (3)
Sb5 ^{vi} —Sr4—Sb4 ^{vi}	93.20 (2)	Sr3—Sb4—Sr5 ^{vii}	76.36 (2)
Sb4—Sr4—Sb4 ^{vi}	46.539 (18)	Sr1—Sb4—Sr5 ^{vii}	73.45 (2)
Sb2 ⁱⁱ —Sr4—Sr3 ^{vi}	58.277 (18)	Sr4—Sb4—Sr5 ^{vii}	69.68 (2)
Sb1—Sr4—Sr3 ^{vi}	120.14 (3)	Sr2—Sb4—Sr5 ^{vii}	69.94 (2)
Sb5 ^{vi} —Sr4—Sr3 ^{vi}	56.052 (19)	Sr2 ^{vi} —Sb4—Sr5 ^{vii}	139.57 (3)
Sb4—Sr4—Sr3 ^{vi}	90.09 (2)	Sr4 ^{vi} —Sb4—Sr5 ^{vii}	142.60 (3)

Sb4 ^{vi} —Sr4—Sr3 ^{vi}	50.294 (18)	Sb4 ^{vi} —Sb4—Sr5 ^{xi}	120.45 (2)
Sb2 ⁱⁱ —Sr4—Sr3 ⁱⁱ	126.62 (3)	Sr3—Sb4—Sr5 ^{xi}	71.66 (2)
Sb1—Sr4—Sr3 ⁱⁱ	56.65 (2)	Sr1—Sb4—Sr5 ^{xi}	74.31 (2)
Sb5 ^{vi} —Sr4—Sr3 ⁱⁱ	94.16 (2)	Sr4—Sb4—Sr5 ^{xi}	141.95 (3)
Sb4—Sr4—Sr3 ⁱⁱ	119.38 (3)	Sr2—Sb4—Sr5 ^{xi}	139.55 (3)
Sb4 ^{vi} —Sr4—Sr3 ⁱⁱ	148.70 (3)	Sr2 ^{vi} —Sb4—Sr5 ^{xi}	67.85 (2)
Sr3 ^{vi} —Sr4—Sr3 ⁱⁱ	149.77 (3)	Sr4 ^{vi} —Sb4—Sr5 ^{xi}	68.76 (2)
Sb2 ⁱⁱ —Sr4—In1 ^{viii}	136.56 (3)	Sr5 ^{vii} —Sb4—Sr5 ^{xi}	115.834 (14)
Sb1—Sr4—In1 ^{viii}	45.916 (16)	In1—Sb5—Sr5 ^{xi}	68.55 (2)
Sb5 ^{vi} —Sr4—In1 ^{viii}	45.685 (15)	In1—Sb5—Sr1 ^x	123.97 (2)
Sb4—Sr4—In1 ^{viii}	135.19 (3)	Sr5 ^{xi} —Sb5—Sr1 ^x	136.52 (2)
Sb4 ^{vi} —Sr4—In1 ^{viii}	109.33 (2)	In1—Sb5—Sr6 ^{ix}	71.51 (2)
Sr3 ^{vi} —Sr4—In1 ^{viii}	97.15 (2)	Sr5 ^{xi} —Sb5—Sr6 ^{ix}	139.88 (2)
Sr3 ⁱⁱ —Sr4—In1 ^{viii}	57.947 (17)	Sr1 ^x —Sb5—Sr6 ^{ix}	66.94 (2)
Sb2 ⁱⁱ —Sr4—Sb3 ^{xi}	82.68 (2)	In1—Sb5—Sr3 ^{iv}	73.754 (18)
Sb1—Sr4—Sb3 ^{xi}	101.02 (2)	Sr5 ^{xi} —Sb5—Sr3 ^{iv}	79.58 (2)
Sb5 ^{vi} —Sr4—Sb3 ^{xi}	78.28 (2)	Sr1 ^x —Sb5—Sr3 ^{iv}	67.577 (18)
Sb4—Sr4—Sb3 ^{xi}	140.45 (3)	Sr6 ^{ix} —Sb5—Sr3 ^{iv}	85.992 (18)
Sb4 ^{vi} —Sr4—Sb3 ^{xi}	162.89 (3)	In1—Sb5—Sr4 ^{vi}	76.562 (19)
Sr3 ^{vi} —Sr4—Sb3 ^{xi}	113.45 (2)	Sr5 ^{xi} —Sb5—Sr4 ^{vi}	77.52 (2)
Sr3 ⁱⁱ —Sr4—Sb3 ^{xi}	47.883 (17)	Sr1 ^x —Sb5—Sr4 ^{vi}	142.88 (2)
In1 ^{viii} —Sr4—Sb3 ^{xi}	75.34 (2)	Sr6 ^{ix} —Sb5—Sr4 ^{vi}	96.94 (2)
Sb2 ⁱⁱ —Sr4—Sr3	56.602 (18)	Sr3 ^{iv} —Sb5—Sr4 ^{vi}	147.51 (2)
Sb1—Sr4—Sr3	122.18 (3)	In1—Sb5—Sr3	134.79 (2)
Sb5 ^{vi} —Sr4—Sr3	150.04 (3)	Sr5 ^{xi} —Sb5—Sr3	75.94 (2)
Sb4—Sr4—Sr3	49.353 (18)	Sr1 ^x —Sb5—Sr3	101.00 (2)
Sb4 ^{vi} —Sr4—Sr3	87.23 (2)	Sr6 ^{ix} —Sb5—Sr3	139.64 (2)
Sr3 ^{vi} —Sr4—Sr3	103.91 (2)	Sr3 ^{iv} —Sb5—Sr3	126.475 (18)
Sr3 ⁱⁱ —Sr4—Sr3	100.919 (19)	Sr4 ^{vi} —Sb5—Sr3	69.05 (2)
In1 ^{viii} —Sr4—Sr3	158.65 (2)	In1—Sb5—Sr2 ^{xi}	123.18 (2)
Sb3 ^{xi} —Sr4—Sr3	92.84 (2)	Sr5 ^{xi} —Sb5—Sr2 ^{xi}	143.65 (2)
Sb2 ⁱⁱ —Sr4—Sr5 ^{vii}	119.86 (2)	Sr1 ^x —Sb5—Sr2 ^{xi}	69.65 (2)
Sb1—Sr4—Sr5 ^{vii}	59.208 (19)	Sr6 ^{ix} —Sb5—Sr2 ^{xi}	65.912 (19)
Sb5 ^{vi} —Sr4—Sr5 ^{vii}	145.92 (3)	Sr3 ^{iv} —Sb5—Sr2 ^{xi}	135.39 (2)
Sb4—Sr4—Sr5 ^{vii}	57.395 (18)	Sr4 ^{vi} —Sb5—Sr2 ^{xi}	73.244 (19)
Sb4 ^{vi} —Sr4—Sr5 ^{vii}	96.50 (2)	Sr3—Sb5—Sr2 ^{xi}	73.76 (2)
Sr3 ^{vi} —Sr4—Sr5 ^{vii}	146.27 (3)	Sb1 ^{vi} —In1—Sb1 ^{xix}	97.92 (3)
Sr3 ⁱⁱ —Sr4—Sr5 ^{vii}	62.03 (2)	Sb1 ^{vi} —In1—Sb5	107.767 (15)
In1 ^{viii} —Sr4—Sr5 ^{vii}	100.44 (2)	Sb1 ^{xix} —In1—Sb5	109.632 (15)
Sb3 ^{xi} —Sr4—Sr5 ^{vii}	98.80 (2)	Sb1 ^{vi} —In1—Sb5 ^{xvi}	109.632 (15)
Sr3—Sr4—Sr5 ^{vii}	63.297 (19)	Sb1 ^{xix} —In1—Sb5 ^{xvi}	107.768 (15)

supplementary materials

Sb2 ⁱⁱ —Sr4—Sr5 ^{ix}	119.92 (2)	Sb5—In1—Sb5 ^{xvi}	121.55 (3)
Sb1—Sr4—Sr5 ^{ix}	58.662 (19)	Sb1 ^{vi} —In1—Sr5 ^{xi}	71.52 (2)
Sb5 ^{vi} —Sr4—Sr5 ^{ix}	49.929 (19)	Sb1 ^{xix} —In1—Sr5 ^{xi}	67.92 (2)
Sb4—Sr4—Sr5 ^{ix}	97.03 (2)	Sb5—In1—Sr5 ^{xi}	61.189 (19)
Sb4 ^{vi} —Sr4—Sr5 ^{ix}	58.800 (18)	Sb5i—In1—Sr5i	175.69 (2)
Sr3 ^{vi} —Sr4—Sr5 ^{ix}	61.65 (2)	Sb1i—In1—Sr5i	67.92 (2)
Sr3 ⁱⁱ —Sr4—Sr5 ^{ix}	104.92 (2)	Sb1i—In1—Sr5i	71.52 (2)
In1 ^{viii} —Sr4—Sr5 ^{ix}	50.828 (15)	Sb5—In1—Sr5i	175.69 (2)
Sb3 ^{xi} —Sr4—Sr5 ^{ix}	121.84 (2)	Sb5i—In1—Sr5i	61.190 (19)
Sr3—Sr4—Sr5 ^{ix}	145.18 (3)	Sr5i—In1—Sr5i	116.30 (4)
Sr5 ^{vii} —Sr4—Sr5 ^{ix}	109.80 (3)	Sb1i—In1—Sr6i	131.039 (16)
Sb3 ^v —Sr5—Sb5 ^v	172.93 (3)	Sb1i—In1—Sr6i	131.039 (16)
Sb3 ^v —Sr5—In1 ^{xii}	125.08 (3)	Sb5—In1—Sr6i	60.776 (17)
Sb5 ^v —Sr5—In1 ^{xii}	50.264 (19)	Sb5i—In1—Sr6i	60.775 (17)
Sb3 ^v —Sr5—Sb1 ^{xiii}	93.22 (2)	Sr5i—In1—Sr6i	121.848 (18)
Sb5 ^v —Sr5—Sb1 ^{xiii}	86.23 (2)	Sr5i—In1—Sr6i	121.848 (18)
In1 ^{xii} —Sr5—Sb1 ^{xiii}	47.861 (14)	Sb1i—In1—Sr3i	60.794 (16)
Sb3 ^v —Sr5—Sb4 ^{xiv}	92.45 (2)	Sb1i—In1—Sr3i	142.55 (2)
Sb5 ^v —Sr5—Sb4 ^{xiv}	93.55 (2)	Sb5—In1—Sr3i	106.35 (2)
In1 ^{xii} —Sr5—Sb4 ^{xiv}	97.74 (2)	Sb5i—In1—Sr3i	59.400 (16)
Sb1 ^{xiii} —Sr5—Sb4 ^{xiv}	62.555 (16)	Sr5i—In1—Sr3i	123.881 (18)
Sb3 ^v —Sr5—Sb1 ^{xiv}	85.95 (2)	Sr5i—In1—Sr3i	71.844 (18)
Sb5 ^v —Sr5—Sb1 ^{xiv}	98.49 (2)	Sr6i—In1—Sr3i	76.528 (16)
In1 ^{xii} —Sr5—Sb1 ^{xiv}	148.75 (3)	Sb1i—In1—Sr3i	142.55 (2)
Sb1 ^{xiii} —Sr5—Sb1 ^{xiv}	145.45 (2)	Sb1i—In1—Sr3i	60.794 (17)
Sb4 ^{xiv} —Sr5—Sb1 ^{xiv}	82.951 (18)	Sb5—In1—Sr3i	59.401 (16)
Sb3 ^v —Sr5—Sb1 ^{xv}	90.67 (2)	Sb5i—In1—Sr3i	106.35 (2)
Sb5 ^v —Sr5—Sb1 ^{xv}	82.44 (2)	Sr5i—In1—Sr3i	71.844 (18)
In1 ^{xii} —Sr5—Sb1 ^{xv}	46.585 (14)	Sr5i—In1—Sr3i	123.881 (18)
Sb1 ^{xiii} —Sr5—Sb1 ^{xv}	72.325 (16)	Sr6i—In1—Sr3i	76.528 (16)
Sb4 ^{xiv} —Sr5—Sb1 ^{xv}	134.87 (2)	Sr3i—In1—Sr3i	153.06 (3)
Sb1 ^{xiv} —Sr5—Sb1 ^{xv}	142.17 (2)	Sb1i—In1—Sr4i	134.58 (2)
Sb3 ^v —Sr5—Sb4 ^v	87.26 (2)	Sb1i—In1—Sr4i	55.642 (15)
Sb5 ^v —Sr5—Sb4 ^v	90.21 (2)	Sb5—In1—Sr4i	115.55 (2)
In1 ^{xii} —Sr5—Sb4 ^v	112.67 (2)	Sb5i—In1—Sr4i	57.754 (16)
Sb1 ^{xiii} —Sr5—Sb4 ^v	154.60 (2)	Sr5i—In1—Sr4i	118.359 (18)
Sb4 ^{xiv} —Sr5—Sb4 ^v	142.84 (2)	Sr5i—In1—Sr4i	68.629 (18)
Sb1 ^{xiv} —Sr5—Sb4 ^v	59.942 (15)	Sr6i—In1—Sr4i	83.985 (17)
Sb1 ^{xv} —Sr5—Sb4 ^v	82.274 (16)	Sr3i—In1—Sr4i	115.891 (17)
Sb3 ^v —Sr5—Sr4 ^{xiv}	121.62 (3)	Sr3i—In1—Sr4i	60.955 (16)
Sb5 ^v —Sr5—Sr4 ^{xiv}	65.22 (2)	Sb1i—In1—Sr4i	55.642 (15)

In1 ^{xii} —Sr5—Sr4 ^{xiv}	106.92 (3)	Sb1i—In1—Sr4i	134.58 (2)
Sb1 ^{xiii} —Sr5—Sr4 ^{xiv}	104.82 (2)	Sb5—In1—Sr4i	57.753 (16)
Sb4 ^{xiv} —Sr5—Sr4 ^{xiv}	52.922 (17)	Sb5i—In1—Sr4i	115.55 (2)
Sb1 ^{xiv} —Sr5—Sr4 ^{xiv}	49.300 (17)	Sr5i—In1—Sr4i	68.629 (18)
Sb1 ^{xv} —Sr5—Sr4 ^{xiv}	147.65 (3)	Sr5i—In1—Sr4i	118.359 (18)
Sb4 ^v —Sr5—Sr4 ^{xiv}	96.39 (2)	Sr6i—In1—Sr4i	83.985 (17)
Sb3 ^v —Sr5—Sr2 ^{xv}	56.484 (19)	Sr3i—In1—Sr4i	60.955 (16)
Sb5 ^v —Sr5—Sr2 ^{xv}	116.98 (2)	Sr3i—In1—Sr4i	115.891 (17)
In1 ^{xii} —Sr5—Sr2 ^{xv}	94.85 (2)	Sr4i—In1—Sr4i	167.97 (3)
Sb1 ^{xiii} —Sr5—Sr2 ^{xv}	107.30 (2)		
?—?—?—?	?		

Symmetry codes: (i) $-x+1/2, -y+1/2, z+1/2$; (ii) $x+1/2, -y+1/2, z$; (iii) $x+1/2, y-1/2, z+1/2$; (iv) $x-1/2, -y+1/2, z$; (v) $-x+1, y, z+1/2$; (vi) $-x+1, -y, z$; (vii) $-x+3/2, -y+1/2, z-1/2$; (viii) $x+1, y, z$; (ix) $x, -y, z-1/2$; (x) $-x+1/2, -y+1/2, z-1/2$; (xi) $-x+1, y, z-1/2$; (xii) $x+1, -y, z+1/2$; (xiii) $-x+2, y, z+1/2$; (xiv) $-x+3/2, -y+1/2, z+1/2$; (xv) $x, -y, z+1/2$; (xvi) $-x, -y, z$; (xvii) $-x, y, z+1/2$; (xviii) $-x+1/2, y-1/2, z$; (xix) $x-1, y, z$; (xx) $x-1, -y, z-1/2$; (xxi) $-x+2, y, z-1/2$; (xxii) $-x+1/2, y+1/2, z$; (xxiii) $x-1/2, y+1/2, z-1/2$.

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
?—? \cdots ?	?	?	?	?

Fig. 1

