

Redetermination of the crystal structure of  
 $\text{K}_2\text{Hg}(\text{SCN})_4$ 

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Single crystals of  $\text{K}_2\text{Hg}(\text{SCN})_4$  [dipotassium tetrathiocyanatomercurate(II)] were grown from aqueous solutions of potassium thiocyanate and mercury(II) thiocyanate and studied by single-crystal X-ray diffraction. In comparison with the previously reported structure model [Zvonkova (1952). *Zh. Fiz. Khim.* **26**, 1798–1803], all atoms in the crystal structure were located, with lattice parameters and fractional coordinates determined to a much higher precision. In the (crystal) structure, the  $\text{Hg}^{\text{II}}$  atom is located on a twofold rotation axis and is coordinated in the form of a distorted tetrahedron by four S atoms of the thiocyanate anions. The  $\text{K}^+$  cation shows a coordination number of eight.

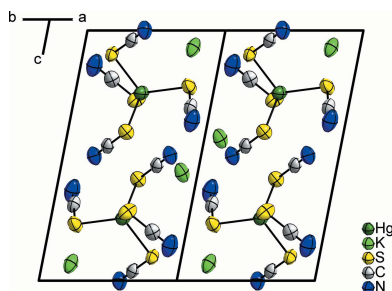
## 1. Chemical context

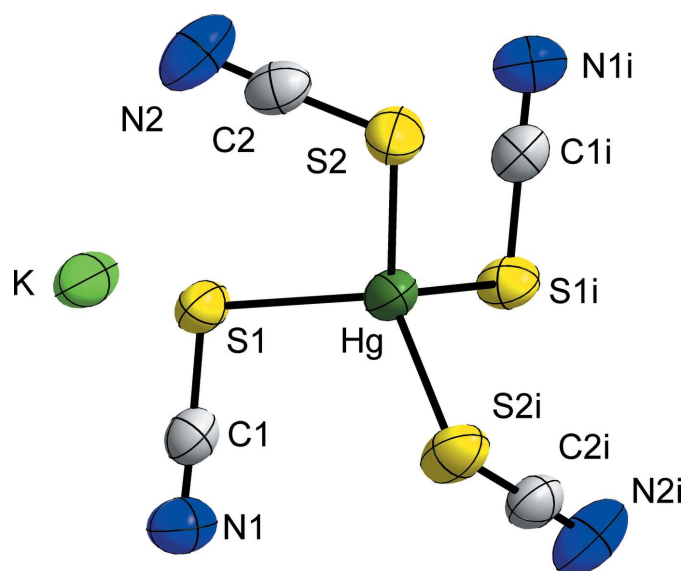
In search for suitable educts for fluorination we thought that  $\text{K}_2\text{Hg}(\text{SCN})_4$  would be a well-suited candidate. Once we had obtained the compound, we noticed that the original structure determination (Zvonkova, 1952) was of low precision with the light atoms (C and N) not determined, so we redetermined the crystal structure to much higher precision and accuracy.

$\text{K}_2\text{Hg}(\text{SCN})_4$  was first synthesized in 1901 (Rosenheim & Cohn, 1901) by adding an aqueous solution of potassium thiocyanate to a boiling solution of mercury(II) thiocyanate and crystallization upon cooling to room temperature. The crystal structure has been known since 1952 (Zvonkova, 1952) and IR spectra were first measured in 1962 (Tramer, 1962). Related compounds of the type  $\text{A}_2\text{Hg}(\text{SCN})_4$  with  $A = \text{Rb}$ ,  $\text{Cs}$ ,  $\text{NH}_4$ ,  $\text{NMe}_4$  are also known (Larbot & Beauchamp, 1973; Tramer, 1962). The  $\text{Hg}^{\text{II}}$  atom in  $\text{K}_2\text{Hg}(\text{SCN})_4$  is coordinated in the form of a distorted tetrahedron by four S atoms in a fashion similar to the  $\text{Hg}^{\text{II}}$  atom in the structure of  $\text{CoHg}(\text{SCN})_4$  (Jefferey & Rose, 1968). Such tetrahedrally coordinated  $\text{Hg}^{\text{II}}$  atoms are also known, for example, for the halide and pseudo-halide compounds  $\text{A}_2\text{HgX}_4$ , viz.  $\text{Cs}_2\text{HgBr}_4$  (Pakhomov *et al.*, 1978; Altermatt *et al.*, 1984; Pinheiro *et al.*, 1998),  $\text{Cs}_2\text{HgCl}_4$  (Linde *et al.*, 1983; Pakhomov *et al.* 1992*a,b*; Bagautdinov & Brown, 2000),  $\text{Cs}_2\text{HgI}_4$  (Zandbergen *et al.*, 1979; Pakhomov & Fedorov, 1973),  $\text{K}_2\text{Hg}(\text{CN})_4$  (Gerlach & Powell, 1986; Dickinson, 1922) and  $\text{Rb}_2\text{Hg}(\text{CN})_4$  (Klüfers *et al.*, 1981).

## 2. Structural commentary

The lattice parameters obtained by our room-temperature single-crystal structure determination (Table 1) agree with those obtained previously ( $a = 11.04$ ,  $b = 9.22$ ,  $c = 13.18$  Å,  $\beta = 106.30^\circ$ ,  $Z = 4$ ; Zvonkova, 1952).  $\text{K}_2\text{Hg}(\text{SCN})_4$  crystallizes in





**Figure 1**  
A section of the crystal structure of  $\text{K}_2\text{Hg}(\text{SCN})_4$ , showing the  $[\text{Hg}(\text{SCN})_4]^{2-}$  anion and the  $\text{K}^+$  cation. Displacement ellipsoids are shown at the 70% probability level at 293 K. [Symmetry code: (i)  $-x, y, \frac{1}{2} - z$ ].

the monoclinic crystal system in space group  $C2/c$  (No. 15). The  $\text{Hg}^{\text{II}}$  atom is located on a twofold rotation axis (Wyckoff position 4e) and is coordinated in the form of a distorted tetrahedron by four S atoms of the thiocyanate anions (Fig. 1). The S–Hg–S angles are in the range  $105.02(2)$ – $114.67(3)^\circ$  and the Hg–S distances are 2.5380 (8) and 2.5550 (7) Å, both in good agreement with the previously reported data (S–Hg–S angle:  $102$ – $118^\circ$ , Hg–S distance: 2.54 (2); Zvonkova, 1952). The Hg–S distance is slightly longer than those of the sixfold-coordinated  $\text{Hg}^{\text{II}}$  atom in  $\text{Hg}(\text{SCN})_2$  [2.381 (6) Å] (Beauchamp & Goutier, 1972) and lies within the range of Hg–S distances [2.3954 (11)–2.7653 (6) Å] for the threefold coordinated  $\text{Hg}^{\text{II}}$  atom in  $\text{KHg}(\text{SCN})_3$  (Weil & Häusler, 2014).

As may be expected, the two unique  $\text{SCN}^-$  anions are almost linear [ $178.0(3)$ ,  $178.2(3)^\circ$ ], and the angles are comparable with those reported for  $\text{Hg}(\text{SCN})_2$  [ $177.5(13)^\circ$ ; Beauchamp & Goutier, 1972] or  $\text{KHg}(\text{SCN})_3$  [ $176.41(4)$ – $179.8(3)^\circ$ ; Weil & Häusler, 2014]. The S–C [1.656 (3), 1.665 (3) Å] and C–N [1.153 (5), 1.152 (4) Å] distances are comparable as well [S–C: 1.62 (2), C–N: 1.18 (3) Å] (Beauchamp & Goutier, 1972) [S–C: 1.657 (4)–1.675 (3) Å, C–N: 1.140 (4)–1.145 (5) Å] (Weil & Häusler, 2014). The Hg–S–C angles in the title salt are  $98.59(10)$  and  $97.06(10)^\circ$ , respectively. In comparison with the coordination polyhedron of the  $\text{Hg}^{\text{II}}$  atom and the structural feature of the  $\text{SCN}^-$  anions in  $\text{CoHg}(\text{SCN})_4$  [Hg–S: 2.558–2.614 Å, S–C: 1.635–1.720 Å, C–N: 1.200–1.322 Å, S–Hg–S angles:  $105.1(1)$ ,  $108.7(1)^\circ$ , Hg–S–C angle:  $97.3(5)^\circ$ ] (Jefferey & Rose, 1968), the respective angles and distances of the complex  $[\text{Hg}(\text{SCN})_4]^{2-}$  anion presented here agree well. In total, a  $[\text{Hg}(\text{SCN})_4]^{2-}$  anion is surrounded by twelve potassium atoms.

The  $\text{K}^+$  cation shows a coordination number of eight, with disparate bond lengths that can be associated with a  $[4 + 3 + 1]$

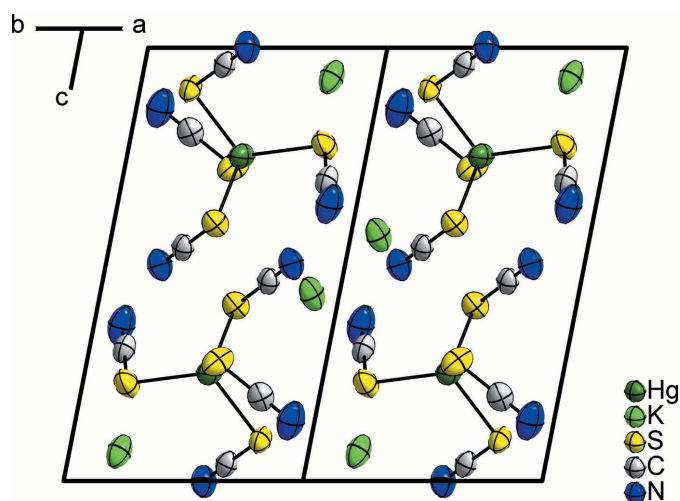
coordination. Four K–N distances are in the range 2.816 (4)–3.031 (5) Å, three K–S distances are in the range 3.4466 (11)–3.5315 (12) Å and there is one very long K–N distance of 3.793 (5) Å. Therefore, the resulting coordination polyhedron is of an odd shape. The  $\text{K}^+$  cation is coordinated in total by five  $[\text{Hg}(\text{SCN})_4]^{2-}$  units, three of these in a monodentate manner (two *via* N atoms and one *via* the S atom of the thiocyanate anions) and the other two in a bidentate mode (*via* the N and S atoms of neighboring thiocyanate anions). Overall, a complex three-dimensional framework results. The crystal structure of the title compound is shown in Fig. 2.

### 3. Synthesis and crystallization

Potassium tetrathiocyanatomercurate(II) was synthesized by slowly adding a potassium thiocyanate solution (2.076 g, 21.36 mmol in 10 ml  $\text{H}_2\text{O}$ ) to a boiling solution of mercury(II) thiocyanate (3.176 g, 10.03 mmol in 10 ml  $\text{H}_2\text{O}$ ). After the formed mercury sulfide had been filtered off through a Büchner funnel, the solution was concentrated on a hot plate until crystallization set in. The crystallized product was collected on a Büchner funnel and the filtrate was allowed to stand at room temperature until crystals of much better quality were obtained. A selected colorless single crystal was investigated by X-ray diffraction. Mercury(II) thiocyanate was prepared as reported previously (Hermes, 1866) using mercury(II) nitrate and potassium thiocyanate and was recrystallized out of ethanol.

### 4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. As a starting model for the structure refinement, the atomic coordinates of the previously reported  $\text{K}_2\text{Hg}(\text{SCN})_4$  structure model were used (Zvonkova,



**Figure 2**  
The crystal structure of  $\text{K}_2\text{Hg}(\text{SCN})_4$  viewed along [110]. Displacement ellipsoids are shown at the 70% probability level at 293 K. Bonds involving the  $\text{K}^+$  cation are omitted for clarity.

**Table 1**  
Experimental details.

Crystal data	
Chemical formula	K <sub>2</sub> Hg(SCN) <sub>4</sub>
<i>M<sub>r</sub></i>	511.11
Crystal system, space group	Monoclinic, <i>C2/c</i>
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.8154 (9), 9.3243 (7), 13.3313 (11)
$\beta$ (°)	106.648 (6)
<i>V</i> (Å <sup>3</sup> )	1288.05 (18)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	13.21
Crystal size (mm)	0.24 × 0.15 × 0.12
Data collection	
Diffraction	Stoe <i>IPDS 2T</i>
Absorption correction	Integration ( <i>X-RED32</i> and <i>X-SHAPE</i> ; Stoe & Cie, 2009)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.103, 0.344
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	14009, 2710, 2298
<i>R<sub>int</sub></i>	0.043
( $\sin \theta/\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.798
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.024, 0.053, 1.08
No. of reflections	2710
No. of parameters	70
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	1.15, -0.75

Computer programs: *X-AREA* (Stoe & Cie, 2011), *X-RED* (Stoe & Cie, 2009), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b), *DIAMOND* (Brandenburg, 2015) and *pubCIF* (Westrip, 2010).

1952). The positions of the C and N atoms were located from a difference-Fourier map.

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## supporting information

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## Computing details

Data collection: *X-AREA* (Stoe & Cie, 2011); cell refinement: *X-AREA* (Stoe & Cie, 2011); data reduction: *X-RED* (Stoe & Cie, 2009); program(s) used to solve structure: *SHELXT2014* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *DIAMOND* (Brandenburg, 2015); software used to prepare material for publication: *publCIF* (Westrip, 2010).

## Dipotassium tetrathiocyanatomercurate(II)

## Crystal data

$\text{K}_2\text{Hg}(\text{SCN})_4$	$F(000) = 936$
$M_r = 511.11$	$D_x = 2.636 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 10.8154 (9) \text{ \AA}$	Cell parameters from 25154 reflections
$b = 9.3243 (7) \text{ \AA}$	$\theta = 2.9\text{--}35.0^\circ$
$c = 13.3313 (11) \text{ \AA}$	$\mu = 13.21 \text{ mm}^{-1}$
$\beta = 106.648 (6)^\circ$	$T = 293 \text{ K}$
$V = 1288.05 (18) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.24 \times 0.15 \times 0.12 \text{ mm}$

## Data collection

Stoe IPDS 2T	$T_{\min} = 0.103, T_{\max} = 0.344$
diffractometer	14009 measured reflections
Radiation source: sealed X-ray tube, 12 x 0.4	2710 independent reflections
mm long-fine focus	2298 reflections with $I > 2\sigma(I)$
Plane graphite monochromator	$R_{\text{int}} = 0.043$
Detector resolution: 6.67 pixels $\text{mm}^{-1}$	$\theta_{\max} = 34.6^\circ, \theta_{\min} = 2.9^\circ$
rotation method scans	$h = -17 \rightarrow 17$
Absorption correction: integration	$k = -14 \rightarrow 14$
(X-RED32 and X-SHAPE; Stoe & Cie, 2009)	$l = -21 \rightarrow 21$

## Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.022P)^2 + 1.7P]$
Least-squares matrix: full	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.024$	$(\Delta/\sigma)_{\max} = 0.001$
$wR(F^2) = 0.053$	$\Delta\rho_{\max} = 1.15 \text{ e \AA}^{-3}$
$S = 1.08$	$\Delta\rho_{\min} = -0.75 \text{ e \AA}^{-3}$
2710 reflections	Extinction correction: <i>SHELXL2014</i>
70 parameters	(Sheldrick, 2015b),
0 restraints	$\text{Fc}^* = k\text{Fc}[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: other	Extinction coefficient: 0.0086 (2)
Secondary atom site location: other	

*Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg	0.0000	0.52099 (2)	0.2500	0.03803 (7)
K	0.16185 (7)	1.04695 (8)	0.43195 (7)	0.04817 (17)
S1	0.10639 (7)	0.68302 (8)	0.40531 (6)	0.03720 (14)
S2	0.18135 (7)	0.36527 (10)	0.22498 (7)	0.04701 (18)
C1	-0.0130 (3)	0.6793 (3)	0.4611 (2)	0.0332 (5)
C2	0.3046 (3)	0.4505 (3)	0.3055 (3)	0.0387 (6)
N1	-0.0940 (3)	0.6801 (3)	0.5013 (3)	0.0462 (6)
N2	0.3926 (3)	0.5077 (4)	0.3607 (4)	0.0615 (9)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Hg	0.02612 (7)	0.05275 (11)	0.03471 (8)	0.000	0.00789 (5)	0.000
K	0.0336 (3)	0.0491 (4)	0.0637 (4)	-0.0053 (3)	0.0169 (3)	-0.0164 (3)
S1	0.0294 (3)	0.0399 (3)	0.0426 (3)	-0.0077 (2)	0.0107 (2)	-0.0070 (3)
S2	0.0350 (3)	0.0567 (5)	0.0486 (4)	0.0053 (3)	0.0108 (3)	-0.0162 (3)
C1	0.0307 (11)	0.0271 (11)	0.0399 (12)	-0.0003 (9)	0.0070 (9)	-0.0026 (9)
C2	0.0304 (12)	0.0385 (15)	0.0475 (14)	0.0066 (10)	0.0115 (10)	0.0066 (11)
N1	0.0408 (13)	0.0437 (14)	0.0586 (17)	-0.0011 (11)	0.0215 (12)	-0.0039 (12)
N2	0.0346 (14)	0.0530 (19)	0.087 (3)	0.0011 (12)	0.0023 (14)	0.0011 (16)

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

Hg—S2	2.5380 (8)	K—K <sup>iv</sup>	4.4669 (15)
Hg—S2 <sup>i</sup>	2.5380 (8)	S1—C1	1.665 (3)
Hg—S1 <sup>i</sup>	2.5550 (7)	S1—K <sup>v</sup>	3.5316 (12)
Hg—S1	2.5551 (7)	S2—C2	1.656 (3)
K—N2 <sup>ii</sup>	2.816 (4)	S2—K <sup>viii</sup>	3.4865 (12)
K—N1 <sup>iii</sup>	2.823 (3)	C1—N1	1.152 (4)
K—N1 <sup>iv</sup>	2.860 (3)	C1—K <sup>iv</sup>	3.529 (3)
K—N2 <sup>v</sup>	3.031 (5)	C2—N2	1.153 (5)
K—C2 <sup>vi</sup>	3.408 (3)	C2—K <sup>viii</sup>	3.408 (3)
K—C2 <sup>v</sup>	3.414 (3)	C2—K <sup>v</sup>	3.414 (3)
K—S1	3.4466 (11)	N1—K <sup>ix</sup>	2.823 (3)
K—S2 <sup>vi</sup>	3.4865 (12)	N1—K <sup>iv</sup>	2.860 (3)
K—S1 <sup>v</sup>	3.5315 (12)	N2—K <sup>x</sup>	2.816 (4)
K—C1 <sup>iv</sup>	3.529 (3)	N2—K <sup>v</sup>	3.031 (5)
K—K <sup>vii</sup>	4.3913 (14)		

S2—Hg—S2 <sup>i</sup>	110.21 (4)	S1—K—C1 <sup>iv</sup>	131.89 (5)
S2—Hg—S1 <sup>i</sup>	114.67 (3)	S2 <sup>vi</sup> —K—C1 <sup>iv</sup>	161.89 (6)
S2 <sup>i</sup> —Hg—S1 <sup>i</sup>	105.02 (2)	S1 <sup>v</sup> —K—C1 <sup>iv</sup>	121.11 (5)
S2—Hg—S1	105.02 (2)	N2 <sup>ii</sup> —K—K <sup>vii</sup>	122.43 (8)
S2 <sup>i</sup> —Hg—S1	114.67 (3)	N1 <sup>iii</sup> —K—K <sup>vii</sup>	39.71 (6)
S1 <sup>i</sup> —Hg—S1	107.50 (4)	N1 <sup>iv</sup> —K—K <sup>vii</sup>	39.09 (6)
N2 <sup>ii</sup> —K—N1 <sup>iii</sup>	161.33 (10)	N2 <sup>v</sup> —K—K <sup>vii</sup>	86.73 (7)
N2 <sup>ii</sup> —K—N1 <sup>iv</sup>	83.58 (10)	C2 <sup>vi</sup> —K—K <sup>vii</sup>	117.52 (6)
N1 <sup>iii</sup> —K—N1 <sup>iv</sup>	78.80 (9)	C2 <sup>v</sup> —K—K <sup>vii</sup>	70.39 (6)
N2 <sup>ii</sup> —K—N2 <sup>v</sup>	80.42 (13)	S1—K—K <sup>vii</sup>	159.02 (4)
N1 <sup>iii</sup> —K—N2 <sup>v</sup>	100.55 (9)	S2 <sup>vi</sup> —K—K <sup>vii</sup>	116.01 (3)
N1 <sup>iv</sup> —K—N2 <sup>v</sup>	74.44 (9)	S1 <sup>v</sup> —K—K <sup>vii</sup>	97.01 (3)
N2 <sup>ii</sup> —K—C2 <sup>vi</sup>	91.55 (12)	C1 <sup>iv</sup> —K—K <sup>vii</sup>	53.40 (5)
N1 <sup>iii</sup> —K—C2 <sup>vi</sup>	94.70 (8)	N2 <sup>ii</sup> —K—K <sup>iv</sup>	41.99 (10)
N1 <sup>iv</sup> —K—C2 <sup>vi</sup>	128.94 (9)	N1 <sup>iii</sup> —K—K <sup>iv</sup>	136.17 (7)
N2 <sup>v</sup> —K—C2 <sup>vi</sup>	154.57 (9)	N1 <sup>iv</sup> —K—K <sup>iv</sup>	75.38 (6)
N2 <sup>ii</sup> —K—C2 <sup>v</sup>	98.21 (12)	N2 <sup>v</sup> —K—K <sup>iv</sup>	38.43 (7)
N1 <sup>iii</sup> —K—C2 <sup>v</sup>	81.16 (8)	C2 <sup>vi</sup> —K—K <sup>iv</sup>	129.03 (5)
N1 <sup>iv</sup> —K—C2 <sup>v</sup>	68.68 (8)	C2 <sup>v</sup> —K—K <sup>iv</sup>	56.66 (5)
N2 <sup>v</sup> —K—C2 <sup>v</sup>	19.47 (8)	S1—K—K <sup>iv</sup>	73.46 (2)
C2 <sup>vi</sup> —K—C2 <sup>v</sup>	161.02 (7)	S2 <sup>vi</sup> —K—K <sup>iv</sup>	136.14 (3)
N2 <sup>ii</sup> —K—S1	72.82 (7)	S1 <sup>v</sup> —K—K <sup>iv</sup>	97.61 (3)
N1 <sup>iii</sup> —K—S1	125.84 (7)	C1 <sup>iv</sup> —K—K <sup>iv</sup>	58.43 (5)
N1 <sup>iv</sup> —K—S1	148.83 (6)	K <sup>vii</sup> —K—K <sup>iv</sup>	107.42 (3)
N2 <sup>v</sup> —K—S1	81.66 (7)	C1—S1—Hg	97.06 (10)
C2 <sup>vi</sup> —K—S1	72.91 (5)	C1—S1—K	96.25 (9)
C2 <sup>v</sup> —K—S1	94.40 (6)	Hg—S1—K	133.66 (3)
N2 <sup>ii</sup> —K—S2 <sup>vi</sup>	111.59 (10)	C1—S1—K <sup>v</sup>	102.56 (10)
N1 <sup>iii</sup> —K—S2 <sup>vi</sup>	80.81 (6)	Hg—S1—K <sup>v</sup>	102.38 (3)
N1 <sup>iv</sup> —K—S2 <sup>vi</sup>	146.21 (6)	K—S1—K <sup>v</sup>	117.55 (2)
N2 <sup>v</sup> —K—S2 <sup>vi</sup>	136.13 (7)	C2—S2—Hg	98.59 (10)
C2 <sup>vi</sup> —K—S2 <sup>vi</sup>	27.76 (5)	C2—S2—K <sup>viii</sup>	73.50 (11)
C2 <sup>v</sup> —K—S2 <sup>vi</sup>	133.75 (5)	Hg—S2—K <sup>viii</sup>	109.15 (3)
S1—K—S2 <sup>vi</sup>	63.89 (2)	N1—C1—S1	178.0 (3)
N2 <sup>ii</sup> —K—S1 <sup>v</sup>	127.71 (8)	N1—C1—K <sup>iv</sup>	46.43 (18)
N1 <sup>iii</sup> —K—S1 <sup>v</sup>	68.47 (7)	S1—C1—K <sup>iv</sup>	131.85 (12)
N1 <sup>iv</sup> —K—S1 <sup>v</sup>	123.33 (7)	N2—C2—S2	178.2 (3)
N2 <sup>v</sup> —K—S1 <sup>v</sup>	68.09 (7)	N2—C2—K <sup>viii</sup>	100.5 (3)
C2 <sup>vi</sup> —K—S1 <sup>v</sup>	99.48 (6)	S2—C2—K <sup>viii</sup>	78.74 (12)
C2 <sup>v</sup> —K—S1 <sup>v</sup>	61.72 (5)	N2—C2—K <sup>v</sup>	61.1 (3)
S1—K—S1 <sup>v</sup>	62.45 (2)	S2—C2—K <sup>v</sup>	119.82 (14)
S2 <sup>vi</sup> —K—S1 <sup>v</sup>	72.06 (2)	K <sup>viii</sup> —C2—K <sup>v</sup>	160.38 (10)
N2 <sup>ii</sup> —K—C1 <sup>iv</sup>	71.53 (9)	C1—N1—K <sup>ix</sup>	127.6 (2)
N1 <sup>iii</sup> —K—C1 <sup>iv</sup>	92.39 (7)	C1—N1—K <sup>iv</sup>	116.6 (2)
N1 <sup>iv</sup> —K—C1 <sup>iv</sup>	16.96 (7)	K <sup>ix</sup> —N1—K <sup>iv</sup>	101.20 (9)
N2 <sup>v</sup> —K—C1 <sup>iv</sup>	61.48 (8)	C2—N2—K <sup>x</sup>	149.3 (3)

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$C2^{vi}-K-C1^{iv}$	138.43 (8)	$C2-N2-K^v$	99.4 (3)
$C2^v-K-C1^{iv}$	60.50 (7)	$K^x-N2-K^v$	99.58 (13)

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Symmetry codes: (i)  $-x, y, -z+1/2$ ; (ii)  $x-1/2, y+1/2, z$ ; (iii)  $x+1/2, y+1/2, z$ ; (iv)  $-x, -y+2, -z+1$ ; (v)  $-x+1/2, -y+3/2, -z+1$ ; (vi)  $-x+1/2, y+1/2, -z+1/2$ ; (vii)  $-x+1/2, -y+5/2, -z+1$ ; (viii)  $-x+1/2, y-1/2, -z+1/2$ ; (ix)  $x-1/2, y-1/2, z$ ; (x)  $x+1/2, y-1/2, z$ .