Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

$Cs_{0.49}NbPS_6$

Eunsil Lee, Yonghee Lee and Hoseop Yun*

Division of Energy Systems Research and Department of Chemistry, Ajou University, Suwon 443-749, Republic of Korea
Correspondence e-mail: hsyun@ajou.ac.kr

Received 14 November 2010; accepted 15 December 2010

Key indicators: single-crystal X-ray study; T = 290 K; mean σ(S–S) = 0.001 Å; disorder in main residue; R factor = 0.020; wR factor = 0.047; data-to-parameter ratio = 23.8.

The quaternary thiophosphate, $Cs_{0.49}NbPS_6$, caesium hexathioniobiophosphate(V), has been synthesized by the reactive halide flux method. The title compound is isotypic with $Rb_{0.46}TaPS_6$ and is made up of a bicapped trigonal–biprismatic [Nb_2S_{12}] unit and a tetrahedral [PS_4] group. The [Nb_2S_{12}] units linked by the [PS_4] tetrahedra form infinite chains, yielding a three-dimensional network with rather large van der Waals gaps along the c axis in which the disordered Cs^+ ions reside. The electrons released by the Cs atoms are transferred to the pairwise niobium metal site and there are substantial intermetallic Nb—Nb bonding interactions. This leads to a significant decrease of the intermetallic distance in the title compound compared to that in $TaPS_6$. The classical charge balance of the title compound may be represented as $[Cs^+]_{0.49}[Nb^{4.51+}][P^{5+}][S^{2-}]_4[S_2^{2-}]$.

Related literature

For the synthesis and structural characterization of $TaPS_6$, see: Fiechter *et al.* (1980). For the related quaternary alkali metal thiophosphates, see: $K_{0.38}TaPS_6$ and $Rb_{0.46}TaPS_6$ (Gutzmann *et al.*, 2004*a*) and $A_2Nb_2P_2S_{12}$ (A = K, Rb, Cs; Gieck *et al.*, 2004). Quite a few quaternary alkali metal thiophosphates having similar composition but with different structures have been reported. For compounds with layered structures, see: Gutzmann & Bensch (2003) for $Rb_4Ta_4P_4S_{24}$; Gutzmann *et al.* (2004*b*) for $Cs_4Ta_4P_4S_{24}$ and $Cs_2Ta_2P_2S_{12}$ and Gutzmann *et al.* (2005) for $K_4Ta_4P_4S_{24}$. For $Rb_2Ta_2P_2S_{11}$ with a one-dimensional structure, see: Gutzmann & Bensch (2002).

Experimental

Crystal data

$Cs_{0.49}NbPS_6$
M_r = 380.95
Tetragonal, $I\bar{4}2d$
a = 15.9477 (3) Å
c = 13.2461 (3) Å
V = 3368.88 (11) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 5.08 mm^{-1}
T = 290 K
0.30 × 0.08 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) T_{min} = 0.751, T_{max} = 1.000
16125 measured reflections
1929 independent reflections
1843 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.047
S = 1.06
1929 reflections
81 parameters
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}
Absolute structure: Flack (1983), 851 Friedel pairs
Flack parameter: 0.452 (18)

Table 1
Selected geometric parameters (Å, °).

Nb—S1^{i}	2.5016 (9)	P1—S2	2.0300 (11)
Nb—S6^{ii}	2.5221 (9)	P1—S5^{vii}	2.0413 (10)
Nb—S1^{iii}	2.5238 (8)	P1—S5^{v}	2.0413 (10)
Nb—S6^{iv}	2.5457 (9)	P2—S3^{viii}	2.0353 (10)
Nb—S2	2.5457 (9)	P2—S3^{ix}	2.0353 (10)
Nb—S3	2.5730 (9)	P2—S4^{ix}	2.0519 (11)
Nb—S5^{v}	2.5971 (9)	P2—S4^{viii}	2.0519 (11)
Nb—S4	2.6266 (9)	S1—S1^{x}	2.0302 (17)
Nb—Nb^{vi}	3.1236 (5)	S6—S6^{xi}	2.0264 (17)
P1—S2^{i}	2.0300 (11)		
S2^{i}—P1—S2	109.11 (7)	S2^{i}—P1—S5^{v}	113.21 (4)
S2^{i}—P1—S5^{vii}	102.92 (3)	S2—P1—S5^{v}	102.92 (3)
S2—P1—S5^{vii}	113.21 (4)	S5^{vii}—P1—S5^{v}	115.63 (7)

Symmetry codes: (i) $x, -y+\frac{1}{2}, -z+\frac{1}{4}$; (ii) $-y, -x+\frac{1}{2}, z+\frac{1}{4}$; (iii) $-x, y-\frac{1}{2}, -z+\frac{1}{4}$; (iv) $y, x-\frac{1}{2}, z+\frac{1}{4}$; (v) $y-\frac{1}{2}, -x+\frac{1}{2}, -z+\frac{1}{2}$; (vi) $-x, -y, z$; (vii) $y-\frac{1}{2}, x, z-\frac{1}{4}$; (viii) $y+\frac{1}{2}, -x+\frac{1}{2}, -z+\frac{1}{2}$; (ix) $y+\frac{1}{2}, x, z-\frac{1}{4}$; (x) $-x, -y+1, z$; (xi) $-x+1, -y, z$.

Data collection: *RAPID-AUTO* (Rigaku, 2006); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: locally modified version of *ORTEP* (Johnson, 1965); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was supported by the Priority Research Centers Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (NRF-2010–0029617). Use was made of the X-ray facilities supported by the Ajou University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2311).

References

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Fiechter, S., Kuhs, W. F. & Nitsche, R. (1980). *Acta Cryst.* B**36**, 2217–2220.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Gieck, C., Derstroff, V., Block, T., Felser, C., Regelsky, G., Jepsen, O., Ksenofontov, V., Gütlich, P., Eckert, H. & Tremel, W. (2004). *Chem. Eur. J.* **10**, 382–391.
Gutzmann, A. & Bensch, W. (2002). *Solid State Sci.* **4**, 835–840.
Gutzmann, A. & Bensch, W. (2003). *Solid State Sci.* **5**, 1271–1276.
Gutzmann, A., Näther, C. & Bensch, W. (2004*a*). *Solid State Sci.* **6**, 1155–1162.
Gutzmann, A., Näther, C. & Bensch, W. (2004*b*). *Inorg. Chem.* **43**, 2998–3004.
Gutzmann, A., Näther, C. & Bensch, W. (2005). *Acta Cryst.* E**61**, i20–i22.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.
Rigaku (2006). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2011). E**67**, i4 [**doi:10.1107/S1600536810052724**]

$Cs_{0.49}NbPS_6$

E. Lee, Y. Lee and H. Yun

Comment

During an effort to find a new phase in the A_xMPS_6 family (A=alkali metals; *M*=Ta, Nb), a new compound was isolated. Here we report the synthesis and structure of the new quaternary thiophosphates, $Cs_{0.49}NbPS_6$.

The title compound is isostructural with the previously reported $Rb_{0.46}TaPS_6$ (Gutzmann *et al.*, 2004*a*). The structure of $Cs_{0.49}NbPS_6$ is also very similar to that of $ANb_2P_2S_{12}$ (A=K, Rb, and Cs, Gieck *et al.*, 2004) prepared from alkali metal sulfide fluxes. The only difference between them lies in the distribution of the alkali metals. There are two crystallographically independent sites for Cs atoms in $ANb_2P_2S_{12}$, while we were able to find only one in $Cs_{0.49}NbPS_6$.

The structure of $Cs_{0.49}NbPS_6$ is made up of the bicapped trigonal biprismatic [Nb_2S_{12}] unit and the tetrahedral [PS_4] group. The niobium atom is coordinated by eight sulfur atoms in a distorted bicapped trigonal prismatic arrangement. Two NbS_8 prisms share a rectangular face to form the [Nb_2S_{12}] dimeric core. Four sulfur atoms sharing rectangular prism faces are in pairs with two disulfide ions, $(S—S)^{2-}$. Each one of the capping sulfur atoms and one of the sulfur atoms at the corner of the [Nb_2S_{12}] unit are bound to a phosphorous atom (Fig. 1). Additional two sulfur atoms from the neighboring [Nb_2S_{12}] units are connected to the phosphorous atoms to complete the [PS_4] tetrahedral coordination. Each [Nb_2S_{12}] unit connects four phosphorous atoms to build up left- and right-handed helices. These helices interwind to each other forming infinite channels along the [001] direction (Fig. 2). The structural array yields rather large channels, where the Cs^+ ions reside. The size of the cations is small compared to the diameter of the large channels and the cations can therefore rattle within the channels as indicated by the high anisotropic displacement parameters.

The Nb—S and P—S distances are in good agreement with those found in other related phases (Gutzmann *et al.*, 2004*b*). The interatomic Nb—Nb distance is 3.124 (1) Å which is similar to those in $K_{0.38}TaPS_6$ (3.142 (2) Å) and $Rb_{0.46}TaPS_6$ (3.1011 (5) Å). These distances are considerably shorter compared to that in $TaPS_6$ (3.361 (1) Å, Fiechter *et al.*, 1980). The electrons released by the Cs atoms are transferred to pair-wise niobium metal sites and there are substantial intermetallic Nb—Nb bonding interactions. Consequently, the classical charge balance of the title compound may be represented as $[Cs^+]_{0.49}[M^{4.51+}][P^{5+}][S^{2-}]_4[S_2^{2-}]$.

Experimental

$Cs_{0.49}NbPS_6$ was prepared by the reaction of elements Nb, P, and S by the reactive halide-flux technique. A combination of the pure elements, Nb powder (CERAC 99.999%), P powder (CERAC 99.5%) and S powder (Aldrich 99.999%) were mixed in a fused silica tube in molar ratio of Nb:*P*:*S*=1:1:6 in the presence of CsCl as flux. The mass ratio of the reactants and the alkali halide flux was 1:2. The tube was evacuated to 0.133 Pa, sealed, and heated gradually (60 K/h) to 973 K, where it was kept for 72 h. The tube was cooled to room temperature at the rate 4 K/h. The excess halide was removed with distilled water and shiny black needle-shaped crystals were obtained. The crystals are stable in air and water. Qualitative analysis of the crystals with an EDAX-equipped SEM indicated the presence of Cs, Nb, P, and S. The composition of the compound was determined by single-crystal X-ray diffraction.

Refinement

(type here to add refinement details)

Figures

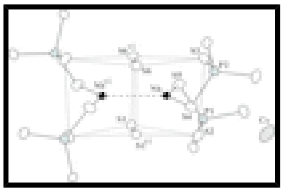

Fig. 1. A perspective view of the bicapped trigonal biprismatic [Nb_2S_{12}] unit and its neighboring tetrahedral [PS_4] groups. The Nb—S bonds have been omitted for clarity, except for the capping S atoms. Displacement ellipsoids are drawn at the 60% probability level. [Symmetry code: (vi) -*x*, -*y*, *z*]

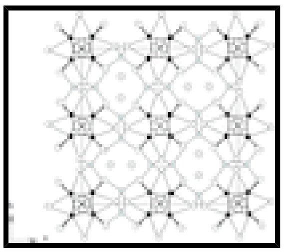

Fig. 2. View of $Cs_{0.49}NbPS_6$ along the **c** axis. Atoms are as marked in Fig. 1.

caesium niobium phosphorus hexasulfide

Crystal data

$Cs_{0.49}NbPS_6$	D_x = 3.004 Mg m^{-3}
M_r = 380.95	Mo *K*α radiation, λ = 0.71073 Å
Tetragonal, $I\bar{4}2d$	Cell parameters from 14367 reflections
Hall symbol: I -4 2bw	θ = 3.3–27.5°
a = 15.9477 (3) Å	μ = 5.08 mm^{-1}
c = 13.2461 (3) Å	*T* = 290 K
V = 3368.88 (11) Å^3	Needle, black
Z = 16	0.30 × 0.08 × 0.06 mm
F(000) = 2860	

Data collection

Rigaku R-AXIS RAPID diffractometer	1843 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.032
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	θ_{max} = 27.5°, θ_{min} = 3.2°
T_{min} = 0.751, T_{max} = 1.000	*h* = −20→20
16125 measured reflections	*k* = −20→20
1929 independent reflections	*l* = −16→17

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2 + 0.1672P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.020$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.047$	$\Delta\rho_{max} = 0.84$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.42$ e Å^{-3}
1929 reflections	Absolute structure: Flack (1983), 851 Friedel pairs
81 parameters	Flack parameter: 0.452 (18)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cs	0.31826 (2)	0.25	0.125	0.04486 (17)	0.974 (2)
Nb	0.066145 (17)	0.072220 (17)	0.24995 (2)	0.01403 (8)	
P1	0.05549 (7)	0.25	0.125	0.0163 (2)	
P2	0.58291 (7)	0.25	0.125	0.0161 (2)	
S1	0.04769 (5)	0.54216 (5)	0.12737 (6)	0.01871 (18)	
S2	0.12931 (6)	0.14853 (5)	0.09924 (7)	0.02128 (18)	
S3	0.14510 (5)	0.15492 (6)	0.38699 (7)	0.0232 (2)	
S4	0.22010 (5)	0.01370 (5)	0.24947 (7)	0.02042 (18)	
S5	0.28529 (5)	0.48732 (5)	0.25169 (7)	0.02144 (19)	
S6	0.45621 (5)	0.04603 (5)	0.12972 (6)	0.01928 (19)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs	0.0218 (2)	0.0690 (3)	0.0438 (2)	0	0	0.0247 (2)
Nb	0.01411 (14)	0.01527 (14)	0.01272 (13)	−0.00014 (9)	−0.00042 (12)	−0.00043 (12)
P1	0.0171 (5)	0.0137 (5)	0.0181 (5)	0	0	0.0005 (5)
P2	0.0191 (5)	0.0140 (5)	0.0153 (5)	0	0	−0.0011 (5)
S1	0.0200 (4)	0.0213 (4)	0.0148 (3)	0.0027 (3)	−0.0025 (4)	−0.0031 (3)
S2	0.0219 (4)	0.0167 (4)	0.0252 (4)	0.0008 (3)	0.0066 (3)	0.0008 (3)
S3	0.0187 (4)	0.0246 (4)	0.0262 (5)	0.0045 (4)	−0.0045 (3)	−0.0115 (4)
S4	0.0200 (4)	0.0236 (4)	0.0177 (4)	0.0059 (3)	−0.0015 (4)	−0.0051 (4)
S5	0.0221 (4)	0.0227 (4)	0.0196 (4)	−0.0066 (3)	0.0028 (4)	−0.0059 (4)
S6	0.0216 (4)	0.0201 (4)	0.0161 (4)	0.0017 (4)	0.0013 (4)	−0.0020 (3)

Geometric parameters (Å, °)

Cs—S2	3.4374 (10)	P1—S2^{i}	2.0300 (11)
Cs—S2^{i}	3.4373 (10)	P1—S2	2.0300 (11)
Cs—S3^{ii}	3.5468 (9)	P1—S5^{xi}	2.0413 (10)
Cs—S3^{iii}	3.5468 (9)	P1—S5^{ix}	2.0413 (10)
Cs—S4^{iv}	3.5646 (9)	P2—S3^{iv}	2.0353 (10)
Cs—S4^{v}	3.5646 (9)	P2—S3^{v}	2.0353 (10)
Cs—S6^{i}	3.9274 (9)	P2—S4^{v}	2.0519 (11)
Cs—S6	3.9274 (9)	P2—S4^{iv}	2.0519 (11)
Cs—S5^{i}	4.1733 (8)	S1—S1^{xii}	2.0302 (17)
Cs—S5	4.1733 (8)	S1—Nb^{i}	2.5016 (9)
Cs—P1	4.1906 (12)	S1—Nb^{xiii}	2.5238 (8)
Cs—P2	4.2206 (13)	S3—P2^{xiv}	2.0353 (10)
Nb—S1^{i}	2.5016 (9)	S3—Cs^{xv}	3.5468 (9)
Nb—S6^{vi}	2.5221 (9)	S4—P2^{xiv}	2.0519 (11)
Nb—S1^{vii}	2.5238 (8)	S4—Cs^{xiv}	3.5646 (9)
Nb—S6^{viii}	2.5457 (9)	S5—P1^{xvi}	2.0413 (10)
Nb—S2	2.5457 (9)	S5—Nb^{xvi}	2.5971 (9)
Nb—S3	2.5730 (9)	S6—S6^{xvii}	2.0264 (17)
Nb—S5^{ix}	2.5971 (9)	S6—Nb^{xviii}	2.5221 (9)
Nb—S4	2.6266 (9)	S6—Nb^{v}	2.5457 (9)
Nb—Nb^{x}	3.1236 (5)		
S2—Cs—S2^{i}	57.52 (3)	S1^{i}—Nb—S2	82.33 (3)
S2—Cs—S3^{ii}	104.92 (2)	S6^{vi}—Nb—S2	154.30 (3)
S2^{i}—Cs—S3^{ii}	91.80 (2)	S1^{vii}—Nb—S2	81.46 (3)
S2—Cs—S3^{iii}	91.80 (2)	S6^{viii}—Nb—S2	157.94 (3)
S2^{i}—Cs—S3^{iii}	104.92 (2)	S1^{i}—Nb—S3	155.09 (3)
S3^{ii}—Cs—S3^{iii}	161.04 (3)	S6^{vi}—Nb—S3	87.62 (3)
S2—Cs—S4^{iv}	151.14 (2)	S1^{vii}—Nb—S3	157.05 (3)
S2^{i}—Cs—S4^{iv}	131.09 (2)	S6^{viii}—Nb—S3	87.58 (3)
S3^{ii}—Cs—S4^{iv}	102.32 (2)	S2—Nb—S3	96.58 (3)
S3^{iii}—Cs—S4^{iv}	59.903 (19)	S1^{i}—Nb—S5^{ix}	125.13 (3)
S2—Cs—S4^{v}	131.09 (2)	S6^{vi}—Nb—S5^{ix}	79.61 (3)
S2^{i}—Cs—S4^{v}	151.14 (2)	S1^{vii}—Nb—S5^{ix}	79.19 (3)
S3^{ii}—Cs—S4^{v}	59.903 (19)	S6^{viii}—Nb—S5^{ix}	125.49 (3)
S3^{iii}—Cs—S4^{v}	102.32 (2)	S2—Nb—S5^{ix}	76.51 (3)
S4^{iv}—Cs—S4^{v}	58.06 (3)	S3—Nb—S5^{ix}	78.13 (3)
S2—Cs—S6^{i}	151.57 (2)	S1^{i}—Nb—S4	81.33 (3)
S2^{i}—Cs—S6^{i}	95.896 (19)	S6^{vi}—Nb—S4	126.93 (3)

$S3^{ii}$—Cs—$S6^{i}$	62.58 (2)	$S1^{vii}$—Nb—S4	127.11 (3)
$S3^{iii}$—Cs—$S6^{i}$	106.020 (19)	$S6^{viii}$—Nb—S4	82.02 (3)
$S4^{iv}$—Cs—$S6^{i}$	53.620 (18)	S2—Nb—S4	78.35 (3)
$S4^{v}$—Cs—$S6^{i}$	67.27 (2)	S3—Nb—S4	74.12 (3)
S2—Cs—S6	95.896 (19)	$S5^{ix}$—Nb—S4	139.76 (3)
$S2^{i}$—Cs—S6	151.57 (2)	$S1^{i}$—Nb—Nb^{x}	51.888 (19)
$S3^{ii}$—Cs—S6	106.020 (19)	$S6^{vi}$—Nb—Nb^{x}	52.29 (2)
$S3^{iii}$—Cs—S6	62.58 (2)	$S1^{vii}$—Nb—Nb^{x}	51.25 (2)
$S4^{iv}$—Cs—S6	67.27 (2)	$S6^{viii}$—Nb—Nb^{x}	51.61 (2)
$S4^{v}$—Cs—S6	53.620 (18)	S2—Nb—Nb^{x}	128.30 (2)
$S6^{i}$—Cs—S6	111.87 (3)	S3—Nb—Nb^{x}	135.12 (2)
S2—Cs—$S5^{i}$	54.738 (19)	$S5^{ix}$—Nb—Nb^{x}	108.56 (2)
$S2^{i}$—Cs—$S5^{i}$	110.88 (2)	S4—Nb—Nb^{x}	111.67 (2)
$S3^{ii}$—Cs—$S5^{i}$	92.93 (2)	$S2^{i}$—P1—S2	109.11 (7)
$S3^{iii}$—Cs—$S5^{i}$	89.45 (2)	$S2^{i}$—P1—$S5^{xi}$	102.92 (3)
$S4^{iv}$—Cs—$S5^{i}$	114.78 (2)	S2—P1—$S5^{xi}$	113.21 (4)
$S4^{v}$—Cs—$S5^{i}$	78.539 (18)	$S2^{i}$—P1—$S5^{ix}$	113.21 (4)
$S6^{i}$—Cs—$S5^{i}$	144.617 (19)	S2—P1—$S5^{ix}$	102.92 (3)
S6—Cs—$S5^{i}$	47.615 (17)	$S5^{xi}$—P1—$S5^{ix}$	115.63 (7)
S2—Cs—S5	110.88 (2)	$S2^{i}$—P1—Cs	54.56 (4)
$S2^{i}$—Cs—S5	54.738 (19)	S2—P1—Cs	54.56 (4)
$S3^{ii}$—Cs—S5	89.45 (2)	$S5^{xi}$—P1—Cs	122.18 (4)
$S3^{iii}$—Cs—S5	92.93 (2)	$S5^{ix}$—P1—Cs	122.18 (4)
$S4^{iv}$—Cs—S5	78.539 (18)	$S3^{iv}$—P2—$S3^{v}$	111.30 (8)
$S4^{v}$—Cs—S5	114.78 (2)	$S3^{iv}$—P2—$S4^{v}$	115.55 (4)
$S6^{i}$—Cs—S5	47.615 (17)	$S3^{v}$—P2—$S4^{v}$	100.12 (3)
S6—Cs—S5	144.616 (19)	$S3^{iv}$—P2—$S4^{iv}$	100.12 (3)
$S5^{i}$—Cs—S5	165.52 (3)	$S3^{v}$—P2—$S4^{iv}$	115.55 (4)
S2—Cs—P1	28.759 (15)	$S4^{v}$—P2—$S4^{iv}$	114.91 (8)
$S2^{i}$—Cs—P1	28.759 (15)	$S3^{iv}$—P2—Cs	124.35 (4)
$S3^{ii}$—Cs—P1	99.482 (14)	$S3^{v}$—P2—Cs	124.35 (4)
$S3^{iii}$—Cs—P1	99.482 (14)	$S4^{v}$—P2—Cs	57.46 (4)
$S4^{iv}$—Cs—P1	150.970 (14)	$S4^{iv}$—P2—Cs	57.46 (4)
$S4^{v}$—Cs—P1	150.970 (14)	$S1^{xii}$—S1—Nb^{i}	66.74 (3)
$S6^{i}$—Cs—P1	124.066 (13)	$S1^{xii}$—S1—Nb^{xiii}	65.60 (3)
S6—Cs—P1	124.066 (13)	Nb^{i}—S1—Nb^{xiii}	76.86 (3)
$S5^{i}$—Cs—P1	82.760 (13)	P1—S2—Nb	91.14 (3)
S5—Cs—P1	82.760 (13)	P1—S2—Cs	96.69 (4)
S2—Cs—P2	151.241 (15)	Nb—S2—Cs	119.61 (3)
$S2^{i}$—Cs—P2	151.241 (15)	$P2^{xiv}$—S3—Nb	93.32 (4)
$S3^{ii}$—Cs—P2	80.518 (14)	$P2^{xiv}$—S3—Cs^{xv}	100.09 (3)

$S3^{iii}$—Cs—P2	80.518 (14)	Nb—S3—Cs^{xv}	157.95 (4)
$S4^{iv}$—Cs—P2	29.030 (14)	$P2^{xiv}$—S4—Nb	91.38 (3)
$S4^{v}$—Cs—P2	29.030 (14)	$P2^{xiv}$—S4—Cs^{xiv}	93.51 (4)
$S6^{i}$—Cs—P2	55.934 (13)	Nb—S4—Cs^{xiv}	115.76 (3)
S6—Cs—P2	55.934 (13)	$P1^{xvi}$—S5—Nb^{xvi}	89.43 (3)
$S5^{i}$—Cs—P2	97.240 (13)	$P1^{xvi}$—S5—Cs	147.09 (5)
S5—Cs—P2	97.240 (13)	Nb^{xvi}—S5—Cs	108.99 (3)
P1—Cs—P2	180	$S6^{xvii}$—S6—Nb^{xviii}	67.04 (3)
$S1^{i}$—Nb—$S6^{vi}$	104.18 (3)	$S6^{xvii}$—S6—Nb^{v}	65.82 (3)
$S1^{i}$—Nb—$S1^{vii}$	47.65 (4)	Nb^{xviii}—S6—Nb^{v}	76.10 (3)
$S6^{vi}$—Nb—$S1^{vii}$	84.90 (3)	$S6^{xvii}$—S6—Cs	170.46 (6)
$S1^{i}$—Nb—$S6^{viii}$	84.86 (3)	Nb^{xviii}—S6—Cs	118.42 (3)
$S6^{vi}$—Nb—$S6^{viii}$	47.14 (4)	Nb^{v}—S6—Cs	106.98 (3)
$S1^{vii}$—Nb—$S6^{viii}$	102.86 (3)		

Symmetry codes: (i) *x*, −*y*+1/2, −*z*+1/4; (ii) −*x*+1/2, −*y*+1/2, *z*−1/2; (iii) −*x*+1/2, *y*, −*z*+3/4; (iv) *y*+1/2, −*x*+1/2, −*z*+1/2; (v) *y*+1/2, *x*, *z*−1/4; (vi) −*y*, −*x*+1/2, *z*+1/4; (vii) −*x*, *y*−1/2, −*z*+1/4; (viii) *y*, *x*−1/2, *z*+1/4; (ix) *y*−1/2, −*x*+1/2, −*z*+1/2; (x) −*x*, −*y*, *z*; (xi) *y*−1/2, *x*, *z*−1/4; (xii) −*x*, −*y*+1, *z*; (xiii) −*x*, *y*+1/2, −*z*+1/4; (xiv) −*y*+1/2, *x*−1/2, −*z*+1/2; (xv) −*x*+1/2, −*y*+1/2, *z*+1/2; (xvi) −*y*+1/2, *x*+1/2, −*z*+1/2; (xvii) −*x*+1, −*y*, *z*; (xviii) −*y*+1/2, −*x*, *z*−1/4.

Fig. 1

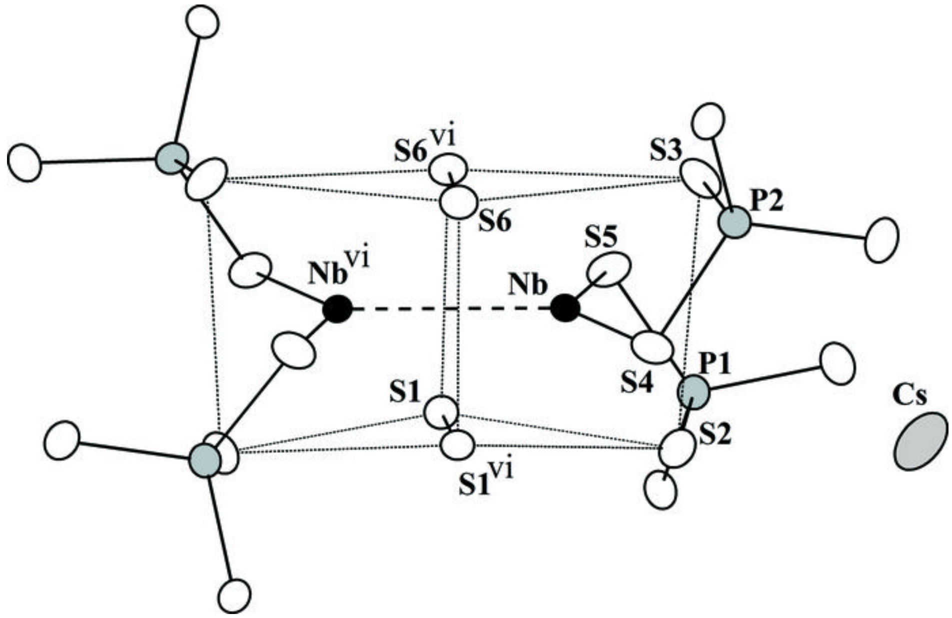

Fig. 2