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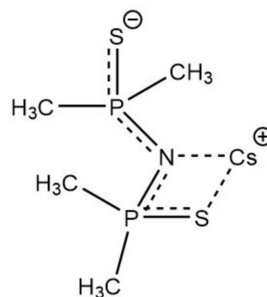
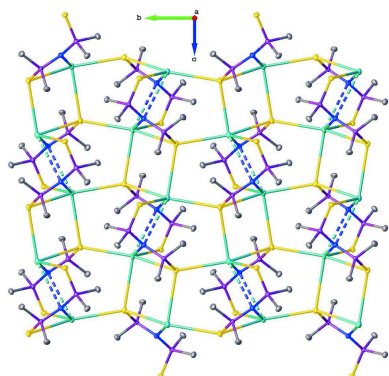
Crystal structure of caesium tetramethyldithioimidodiphosphinate

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In the title crystal, the salt $[\text{CsMe}_2\text{P}(\text{S})\text{NP}(\text{S})\text{Me}_2]$ is self-assembled as an undulating supramolecular two-dimensional polymeric structure, poly $[(\mu_4\text{-tetramethyldithioimidodiphosphinato})\text{caesium}]_n$, which is parallel to the bc plane. The Cs cations are hexacoordinated, being chelated by two thioimidodiphosphinate groups and two sulfur atoms from neighboring ligands. The anions are linked to the Cs cations by $\text{Cs}\cdots\text{S}$ and $\text{Cs}\cdots\text{N}$ electrostatic interactions.

1. Chemical context

Dichalcogenoimidodiphosphinate anions $[\text{R}_2\text{P}(\text{E})\text{NP}(\text{E})\text{R}_2]^-$ ($\text{E} = \text{O}, \text{S}, \text{Se}, \text{Te}$) are versatile complexing reagents with a strong tendency to form inorganic (carbon-free) chelate rings (Haiduc & Silaghi-Dumitrescu, 1986; Cea-Olivares & Muñoz, 1993; Hernández-Arganis *et al.*, 2004; Slawin *et al.*, 1994). The monoanionic ligands have been investigated as ligands for both main-group elements (Silvestru & Drake, 2001; Woollins, 1996) and transition metals (Rudler *et al.*, 1997). The widespread interest in dichalcogenoimidodiphosphinates stems from their potential uses as lanthanide shift reagents (Rudler *et al.*, 1997), industrial catalysts (Leung *et al.*, 2000; Yamazaki *et al.*, 2020), luminescent materials (Ma *et al.*, 2019) as well as in metal extraction processes (du Preez *et al.*, 1992). As part of our ongoing research on dichalcogenoimidodiphosphinate anions, we report herein the synthesis and crystallographic study of the title compound (**I**).



2. Structural commentary

In the asymmetric unit of the title compound (**I**) (Fig. 1), the tetramethyldithioimidodiphosphinate anion is bent with a $\text{P}-\text{N}-\text{P}$ angle of $132.16(6)^\circ$, and chelates the Cs cation through



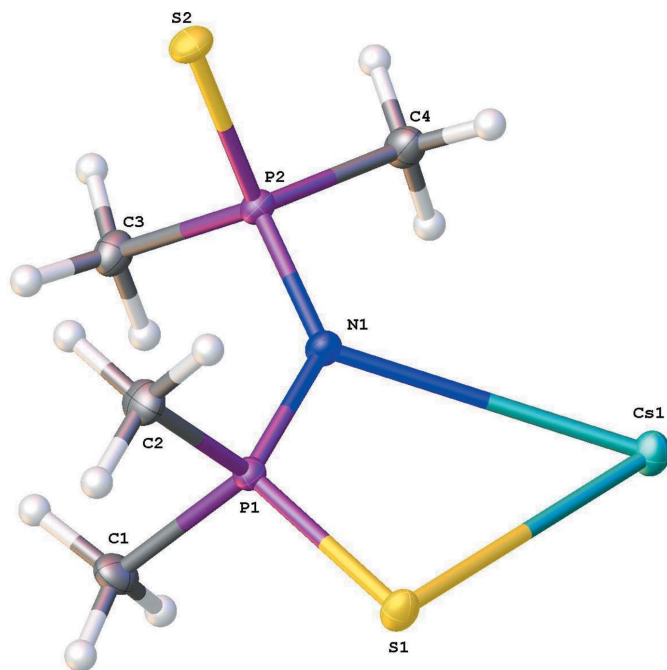


Figure 1
The asymmetric unit of the title compound (**I**), showing the atom-labeling scheme.

$S \cdots Cs \cdots N$ electrostatic interactions [$S \cdots Cs \cdots N = 53.074 (17)^\circ$; $S \cdots Cs = 3.4377 (3) \text{ \AA}$; $N \cdots Cs = 3.2054 (9) \text{ \AA}$]. The bond distances of 2.0003 (4), 1.6075 (10), 1.6179 (10) and 1.9869 (4) \AA for $S1-P1$, $P1-N1$, $N1-P2$ and $P2-S2$, respectively, suggest that the anion is a delocalized system (Cea-Olivares & Nöth, 1987; Churchill *et al.*, 1971). The phosphorus atoms are in an approximately tetrahedral environment, the average bond angles being $S-P-N = 113.9^\circ$, $S-P-C = 109.4^\circ$, and $C-P-C = 103.4^\circ$.

3. Supramolecular features

In the crystal, the salt $[\text{CsMe}_2\text{P}(\text{S})\text{NP}(\text{S})\text{Me}_2]$ (**I**) is self-assembled as an undulating supramolecular 2D polymeric structure, which is parallel to the bc plane (Figs. 2 and 3). The

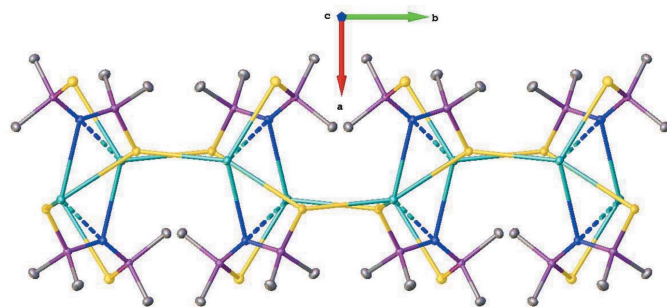


Figure 2
A view along the c axis, showing the undulating two-dimensional polymer structure. Hydrogen atoms were omitted for clarity.

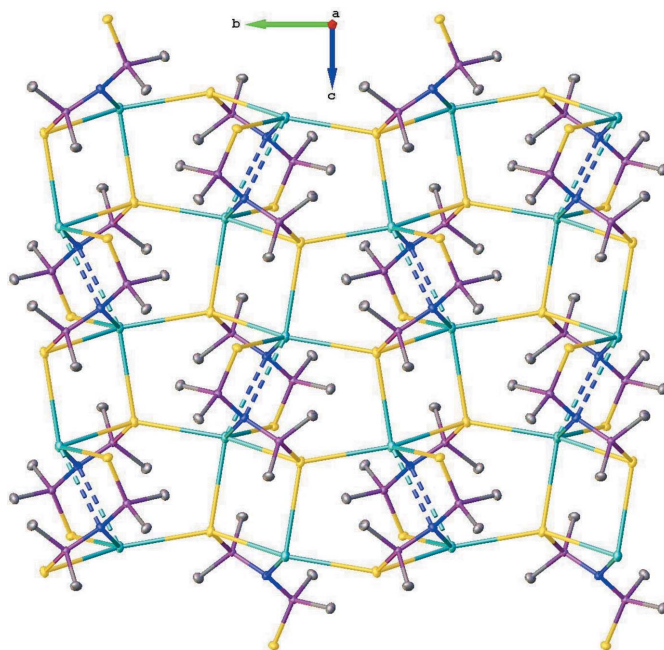


Figure 3
A view along the a axis of the supramolecular two-dimensional polymer structure parallel to the bc plane. Hydrogen atoms were omitted for clarity.

Cs cations are hexacoordinated and linked to four different anions by $Cs \cdots S$ and $Cs \cdots N$ electrostatic interactions (Fig. 4). Analysis of this CsS_4N_2 polyhedron with the *SHAPE 2.1* program (Llunell *et al.*, 2013) gave CShM values of 9.50434 and 8.43874 for a regular octahedron and a trigonal prism,

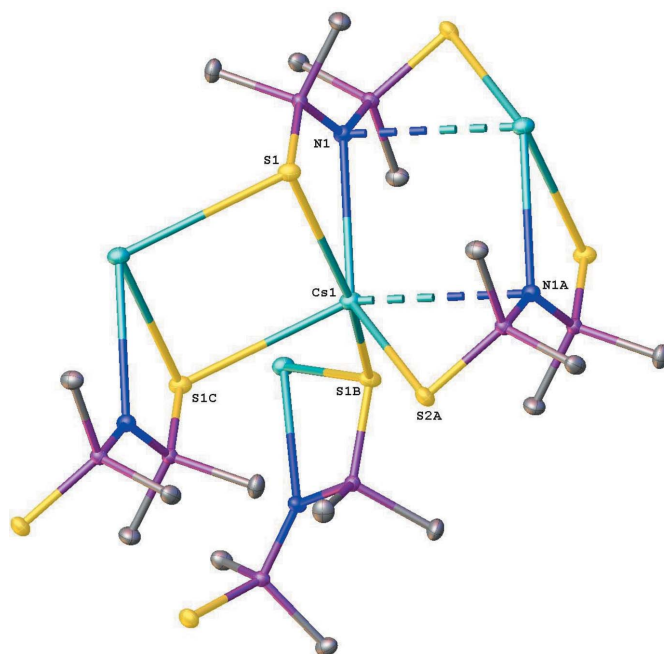


Figure 4
A view of the hexacoordination of the caesium cation. Atoms with the suffix A, B or C are at the symmetry positions A: $1-x, 1-y, 1-z$; B: $1-x, \frac{1}{2}+y, \frac{1}{2}-z$; C: $1-x, 1-y, -z$. Hydrogen atoms were omitted for clarity.

Table 1
Experimental details.

Crystal data	
Chemical formula	[Cs(C ₄ H ₁₂ NP ₂ S ₂)]
<i>M_r</i>	333.12
Crystal system, space group	Monoclinic, <i>P</i> ₂ /c
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.0320 (2), 12.4326 (3), 8.2173 (2)
β (°)	93.8752 (4)
<i>V</i> (Å ³)	1124.48 (4)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	3.89
Crystal size (mm)	0.18 × 0.15 × 0.12
Data collection	
Diffractometer	Bruker <i>SMART</i> APEXII DUO
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2016)
<i>T</i> _{min} , <i>T</i> _{max}	0.100, 0.147
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	15582, 5097, 4791
<i>R</i> _{int}	0.017
(sin θ/λ) _{max} (Å ⁻¹)	0.833
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.017, 0.035, 1.08
No. of reflections	5097
No. of parameters	95
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.58, -0.76

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), and *OLEX2* (Dolomanov *et al.*, 2009).

respectively, meaning that the coordination environment of the cesium atom is highly irregular. These polyhedra interconnect either by sharing vertices or an edge. The Cs⋯S ionic bond distances vary from 3.4377 (3) to 3.4726 (3) Å, which are close to the value of 3.51 Å predicted from the ionic radii (Shannon, 1976). Regarding the N–Cs bond distances, two different distances were determined. One of them is 3.2054 (9) Å, which is close to the value of 3.13 Å predicted from the ionic radii, and the other is 3.651 Å, which is less than the value of 4.4 Å predicted from the van der Waals radii (Batsanov, 2001). Furthermore, five methyl groups are located in a close vicinity of the Cs⁺ cation with the Cs⋯H distance shorter than 4 Å, but only the shortest Cs1⋯H2C(1 – *x*, 1 – *y*, 1 – *z*) distance of 3.269 Å is similar to those observed in [LiCs(HMDS)₂]_∞ and can be labeled as an agostic interaction (Ojeda-Amador *et al.*, 2016). The cyclic motifs Cs₂S₂, Cs₂N₂, Cs₂N₂P₂S₂ in this arrangement possess crystallographic inversion symmetry.

4. Database survey

The current version of the Cambridge Structural Database (Version 2021.1, updated August 2021; Groom *et al.*, 2016) contains only three cesium dichalcogenoimidodiphosphinates, (18C6)CsPh₂P(*E*)NP(*E*)Ph₂ (BENSAP, BENSET and BENSIX for *E* = O, S and Se; Hernández-Arganis *et al.*, 2004). Furthermore, only five compounds each containing two [Me₂P(S)NP(S)Me₂][–] ligands and one *M*²⁺ cation (*M* = Fe, Ni,

Pd, Cd, Co) are included in the database: IMSPF10, IMSPN10, OCANEL, TASXAN and ZACZAE (Churchill & Wormald, 1971; Churchill *et al.*, 1971; Bilic *et al.*, 2000; Ghesner *et al.*, 2005 and Silvestru *et al.*, 1995). The dinuclear species MIWYUM with two [Mn(CO)₃]⁺ cations (Zuniga-Villarreal *et al.*, 2001) is also noteworthy. No compound with [Me₂P(*E*)NP(*E*)Me₂][–] (*E* = O or Se) is included in the database.

5. Synthesis and crystallization

Cs[Me₂P(S)]₂N (**I**) was obtained by the reaction of [Me₂P(S)NHP(S)(Me₂)] with Cs₂CO₃, according to a method previously described (Schmidpeter & Ebeling, 1968) and isolated solvent-free. The salt Cs[Me₂P(S)]₂N was recrystallized by slow evaporation from methanol. The spectroscopic data of the received sample (*vide infra*) coincided with the published ones and are therefore not reported; however, they can be consulted in the above-mentioned reference.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were positioned geometrically (C–H = 0.98 Å) and constrained using the riding-model approximation with *U*_{iso}(H) = 1.5 *U*_{eq}(C).

Acknowledgements

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Crystal structure of caesium tetramethyldithioimidodiphosphinate

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: *ShelXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

Poly[(μ_4 -tetramethyldithioimidodiphosphinato)caesium]

Crystal data

[Cs(C₄H₁₂NP₂S₂)]

$M_r = 333.12$

Monoclinic, $P2_1/c$

$a = 11.0320$ (2) Å

$b = 12.4326$ (3) Å

$c = 8.2173$ (2) Å

$\beta = 93.8752$ (4)°

$V = 1124.48$ (4) Å³

$Z = 4$

$F(000) = 640$

$D_x = 1.968$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4791 reflections

$\theta = 2.4$ – 25.2 °

$\mu = 3.89$ mm⁻¹

$T = 100$ K

Plate, clear light white

$0.18 \times 0.15 \times 0.12$ mm

Data collection

Bruker SMART APEXII DUO
diffractometer

Radiation source: Incoatec ImuS with multilayer
mirrors

Detector resolution: 8.333 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2016)

$T_{\min} = 0.100$, $T_{\max} = 0.147$

15582 measured reflections

5097 independent reflections

4791 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$

$\theta_{\max} = 36.3$ °, $\theta_{\min} = 2.5$ °

$h = -17 \rightarrow 17$

$k = -19 \rightarrow 20$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.017$

$wR(F^2) = 0.035$

$S = 1.08$

5097 reflections

95 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0129P)^2 + 0.2359P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.004$

$\Delta\rho_{\max} = 0.58$ e Å⁻³

$\Delta\rho_{\min} = -0.76$ e Å⁻³

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cs1	0.56629 (2)	0.59017 (2)	0.27106 (2)	0.01538 (2)
S1	0.40180 (2)	0.36434 (2)	0.15753 (4)	0.01505 (5)
S2	0.16545 (3)	0.55491 (2)	0.67865 (3)	0.01535 (5)
P1	0.25673 (2)	0.42906 (2)	0.25349 (3)	0.01072 (5)
P2	0.21826 (2)	0.61338 (2)	0.46982 (3)	0.01115 (5)
N1	0.29485 (8)	0.53396 (8)	0.35928 (11)	0.01287 (16)
C1	0.14280 (11)	0.45999 (10)	0.09220 (14)	0.0180 (2)
H1A	0.1713	0.5193	0.0261	0.027*
H1B	0.0672	0.4811	0.1397	0.027*
H1C	0.1280	0.3964	0.0232	0.027*
C2	0.18262 (11)	0.32802 (10)	0.37023 (15)	0.0181 (2)
H2A	0.1574	0.2678	0.2988	0.027*
H2B	0.1111	0.3595	0.4165	0.027*
H2C	0.2392	0.3021	0.4586	0.027*
C3	0.08798 (10)	0.67113 (10)	0.35577 (14)	0.0165 (2)
H3A	0.1128	0.6988	0.2514	0.025*
H3B	0.0551	0.7301	0.4185	0.025*
H3C	0.0255	0.6158	0.3356	0.025*
C4	0.31966 (11)	0.72634 (9)	0.50889 (15)	0.0169 (2)
H4A	0.3379	0.7596	0.4052	0.025*
H4B	0.3952	0.7012	0.5661	0.025*
H4C	0.2807	0.7794	0.5766	0.025*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs1	0.01350 (3)	0.01249 (3)	0.02027 (4)	-0.00100 (2)	0.00205 (2)	-0.00067 (2)
S1	0.01356 (11)	0.01225 (11)	0.01975 (12)	0.00045 (9)	0.00416 (9)	-0.00285 (9)
S2	0.01700 (12)	0.01704 (12)	0.01254 (11)	0.00079 (10)	0.00488 (9)	0.00192 (9)
P1	0.01031 (10)	0.01168 (11)	0.01021 (11)	-0.00022 (9)	0.00089 (8)	0.00053 (8)
P2	0.01079 (11)	0.01129 (11)	0.01158 (11)	0.00056 (9)	0.00243 (9)	0.00048 (9)
N1	0.0121 (4)	0.0131 (4)	0.0136 (4)	-0.0001 (3)	0.0023 (3)	-0.0024 (3)
C1	0.0179 (5)	0.0217 (5)	0.0138 (5)	0.0031 (4)	-0.0035 (4)	-0.0002 (4)
C2	0.0184 (5)	0.0178 (5)	0.0182 (5)	-0.0051 (4)	0.0030 (4)	0.0026 (4)
C3	0.0139 (4)	0.0177 (5)	0.0180 (5)	0.0024 (4)	0.0024 (4)	0.0046 (4)
C4	0.0167 (5)	0.0149 (5)	0.0193 (5)	-0.0021 (4)	0.0040 (4)	-0.0031 (4)

Geometric parameters (Å, °)

Cs1—S1	3.4377 (3)	P1—C2	1.8090 (12)
Cs1—S1 ⁱ	3.4726 (3)	P2—Cs1 ⁱⁱⁱ	3.9879 (3)
Cs1—S1 ⁱⁱ	3.6077 (3)	P2—N1	1.6179 (10)
Cs1—S2 ⁱⁱⁱ	3.4667 (3)	P2—C3	1.8103 (11)
Cs1—N1 ⁱⁱⁱ	3.6506 (9)	P2—C4	1.8107 (12)
Cs1—N1	3.2054 (9)	N1—Cs1 ⁱⁱⁱ	3.6506 (9)
Cs1—H2A ⁱ	3.8388	C1—H1A	0.9800
Cs1—H2C ⁱⁱⁱ	3.2692	C1—H1B	0.9800
Cs1—H4A	3.5176	C1—H1C	0.9800
Cs1—H4B ^{iv}	3.5628	C2—H2A	0.9800
Cs1—H4B	3.4588	C2—H2B	0.9800
Cs1—H4C ^{iv}	3.7984	C2—H2C	0.9800
S1—Cs1 ^v	3.4726 (3)	C3—H3A	0.9800
S1—Cs1 ⁱⁱ	3.6077 (3)	C3—H3B	0.9800
S1—P1	2.0003 (4)	C3—H3C	0.9800
S2—Cs1 ⁱⁱⁱ	3.4667 (3)	C4—H4A	0.9800
S2—P2	1.9869 (4)	C4—H4B	0.9800
P1—N1	1.6075 (10)	C4—H4C	0.9800
P1—C1	1.8052 (11)		
S1—Cs1—S1 ⁱ	153.276 (4)	H4B—Cs1—H4C ^{iv}	69.4
S1—Cs1—S1 ⁱⁱ	86.999 (7)	H4C ^{iv} —Cs1—H2A ⁱ	109.6
S1 ⁱ —Cs1—S1 ⁱⁱ	89.749 (6)	Cs1 ^v —S1—Cs1 ⁱⁱ	107.659 (7)
S1—Cs1—S2 ⁱⁱⁱ	92.185 (7)	Cs1—S1—Cs1 ^v	135.252 (9)
S1 ⁱⁱ —Cs1—N1 ⁱⁱⁱ	144.629 (15)	Cs1—S1—Cs1 ⁱⁱ	93.001 (7)
S1 ⁱ —Cs1—N1 ⁱⁱⁱ	104.024 (15)	P1—S1—Cs1 ⁱⁱ	117.081 (14)
S1—Cs1—N1 ⁱⁱⁱ	93.707 (15)	P1—S1—Cs1	89.211 (12)
S1 ⁱ —Cs1—H2A ⁱ	52.3	P1—S1—Cs1 ^v	113.760 (14)
S1—Cs1—H2A ⁱ	147.1	P2—S2—Cs1 ⁱⁱⁱ	89.743 (12)
S1 ⁱⁱ —Cs1—H2A ⁱ	68.5	S1—P1—Cs1	60.397 (11)
S1—Cs1—H4A	101.4	N1—P1—Cs1	51.35 (3)
S1 ⁱ —Cs1—H4A	55.0	N1—P1—S1	110.64 (4)
S1—Cs1—H4B ^{iv}	102.3	N1—P1—C1	111.59 (5)
S1—Cs1—H4B	102.3	N1—P1—C2	112.81 (5)
S1 ⁱ —Cs1—H4B ^{iv}	53.8	C1—P1—Cs1	118.41 (4)
S1 ⁱⁱ —Cs1—H4C ^{iv}	69.8	C1—P1—S1	109.40 (4)
S1 ⁱ —Cs1—H4C ^{iv}	74.0	C1—P1—C2	102.71 (6)
S1—Cs1—H4C ^{iv}	80.0	C2—P1—Cs1	138.82 (4)
S2 ⁱⁱⁱ —Cs1—S1 ⁱ	114.494 (7)	C2—P1—S1	109.39 (4)
S2 ⁱⁱⁱ —Cs1—S1 ⁱⁱ	93.387 (7)	S2—P2—Cs1 ⁱⁱⁱ	60.375 (11)
S2 ⁱⁱⁱ —Cs1—N1 ⁱⁱⁱ	51.243 (15)	N1—P2—Cs1 ⁱⁱⁱ	66.26 (3)
S2 ⁱⁱⁱ —Cs1—H2A ⁱ	68.7	N1—P2—S2	117.15 (4)
S2 ⁱⁱⁱ —Cs1—H4A	153.9	N1—P2—C3	112.20 (5)
S2 ⁱⁱⁱ —Cs1—H4B ^{iv}	148.8	N1—P2—C4	103.48 (5)
S2 ⁱⁱⁱ —Cs1—H4C ^{iv}	161.7	C3—P2—Cs1 ⁱⁱⁱ	162.13 (4)
N1—Cs1—S1	53.074 (17)	C3—P2—S2	108.87 (4)

N1—Cs1—S1 ⁱ	105.154 (17)	C3—P2—C4	104.09 (6)
N1—Cs1—S1 ⁱⁱ	114.158 (17)	C4—P2—Cs1 ⁱⁱⁱ	93.37 (4)
N1—Cs1—S2 ⁱⁱⁱ	131.503 (18)	C4—P2—S2	110.14 (4)
N1—Cs1—N1 ⁱⁱⁱ	93.76 (2)	Cs1—N1—Cs1 ⁱⁱⁱ	86.24 (2)
N1 ⁱⁱⁱ —Cs1—H2A ⁱ	94.3	P1—N1—Cs1 ⁱⁱⁱ	100.76 (4)
N1—Cs1—H2A ⁱ	157.3	P1—N1—Cs1	105.60 (4)
N1—Cs1—H2C ⁱⁱⁱ	121.1	P1—N1—P2	132.16 (6)
N1—Cs1—H4A	50.2	P2—N1—Cs1	121.68 (4)
N1—Cs1—H4B ^{iv}	78.0	P2—N1—Cs1 ⁱⁱⁱ	89.80 (4)
N1—Cs1—H4B	50.7	P1—C1—H1A	109.5
N1 ⁱⁱⁱ —Cs1—H4C ^{iv}	145.1	P1—C1—H1B	109.5
N1—Cs1—H4C ^{iv}	55.1	P1—C1—H1C	109.5
H2C ⁱⁱⁱ —Cs1—S1 ⁱ	55.1	H1A—C1—H1B	109.5
H2C ⁱⁱⁱ —Cs1—S1 ⁱⁱ	119.8	H1A—C1—H1C	109.5
H2C ⁱⁱⁱ —Cs1—S1	146.0	H1B—C1—H1C	109.5
H2C ⁱⁱⁱ —Cs1—S2 ⁱⁱⁱ	67.4	P1—C2—H2A	109.5
H2C ⁱⁱⁱ —Cs1—N1 ⁱⁱⁱ	52.3	P1—C2—H2B	109.5
H2C ⁱⁱⁱ —Cs1—H2A ⁱ	51.3	P1—C2—H2C	109.5
H2C ⁱⁱⁱ —Cs1—H4A	89.6	H2A—C2—H2B	109.5
H2C ⁱⁱⁱ —Cs1—H4B	74.0	H2A—C2—H2C	109.5
H2C ⁱⁱⁱ —Cs1—H4B ^{iv}	109.0	H2B—C2—H2C	109.5
H2C ⁱⁱⁱ —Cs1—H4C ^{iv}	126.8	P2—C3—H3A	109.5
H4A—Cs1—S1 ⁱⁱ	109.3	P2—C3—H3B	109.5
H4A—Cs1—N1 ⁱⁱⁱ	105.2	P2—C3—H3C	109.5
H4A—Cs1—H2A ⁱ	107.2	H3A—C3—H3B	109.5
H4A—Cs1—H4B ^{iv}	49.1	H3A—C3—H3C	109.5
H4A—Cs1—H4C ^{iv}	44.4	H3B—C3—H3C	109.5
H4B—Cs1—S1 ⁱⁱ	135.7	Cs1—C4—H4A	63.3
H4B—Cs1—S1 ⁱ	62.8	Cs1—C4—H4B	59.7
H4B ^{iv} —Cs1—S1 ⁱⁱ	60.5	Cs1—C4—H4C	159.4
H4B—Cs1—S2 ⁱⁱⁱ	128.8	P2—C4—Cs1	91.05 (4)
H4B—Cs1—N1 ⁱⁱⁱ	78.7	P2—C4—H4A	109.5
H4B ^{iv} —Cs1—N1 ⁱⁱⁱ	151.7	P2—C4—H4B	109.5
H4B—Cs1—H2A ⁱ	110.6	P2—C4—H4C	109.5
H4B ^{iv} —Cs1—H2A ⁱ	84.9	H4A—C4—H4B	109.5
H4B—Cs1—H4A	26.5	H4A—C4—H4C	109.5
H4B—Cs1—H4B ^{iv}	75.2	H4B—C4—H4C	109.5
H4B ^{iv} —Cs1—H4C ^{iv}	24.8		

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