

Crystal structure of O-isopropyl [bis(trimethylsilyl)amino](*tert*-butylamino)-phosphinothioate

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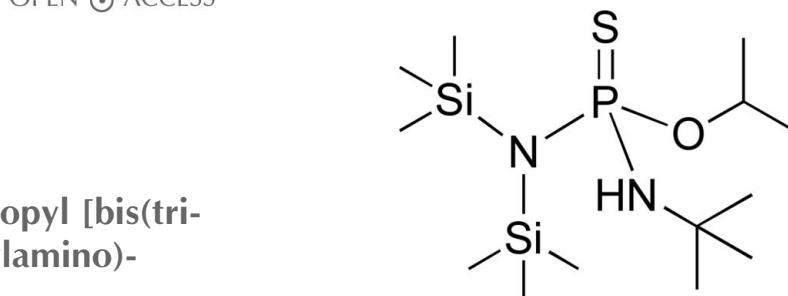
[Bis(trimethylsilyl)amino](*tert*-butylimino)thiophosphorane reacts in benzene with isopropyl alcohol *via* 1,2-addition of an *i*PrO–H bond across the P=N bond, resulting in the title compound, C₁₃H₃₅N₂OPSSi₂. In the molecule, the P atom possesses a distorted tetrahedral environment involving two N atoms from (Me₃Si)₂N– and *t*BuNH– groups, one O atom from an *i*PrO group and one S atom, therefore the molecule has a stereocenter on the P atom but crystal symmetry leads to a racemate. In the crystal, a pair of enantiomers form a centrosymmetric dimer *via* a pair of N–H···S hydrogen bonds.

Keywords: crystal structure; (trimethylsilyl)amino; phosphinothioate; N–H···S hydrogen bonding.

CCDC reference: 1036750

1. Related literature

For details of the synthesis of [bis(trimethylsilyl)amino](*tert*-butylimino)thiophosphorane, see: Scherer & Kuhn (1974). For its chemical reactivity, see: Kovalenko *et al.* (2011a,b,c, 2012); Rusanov *et al.* (1992); Scherer *et al.* (1978). For its applications in catalysis, see: Zhao *et al.* (2014a,b); Goldys & Dixon (2014); Samuel *et al.* (2014); Kawalec *et al.* (2012); Zhang *et al.* (2007).



2. Experimental

2.1. Crystal data

C₁₃H₃₅N₂OPSSi₂
*M*_r = 354.64
 Monoclinic, *P*2₁/*n*
a = 9.942 (3) Å
b = 11.907 (3) Å
c = 17.726 (5) Å
 β = 100.52 (3)°

V = 2063.1 (10) Å³
Z = 4
 Mo *K*α radiation
 μ = 0.35 mm⁻¹
T = 100 K
 0.30 × 0.20 × 0.20 mm

2.2. Data collection

Oxford Xcalibur PX κ -geometry diffractometer with a CCD area detector
 7436 independent reflections
 5938 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.033

36939 measured reflections

2.3. Refinement

R[F² > 2σ(F²)] = 0.041
wR(F²) = 0.115
S = 1.08
 7436 reflections
 184 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max}$ = 0.84 e Å⁻³
 $\Delta\rho_{\min}$ = -0.34 e Å⁻³

Table 1
 Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
N2–H2···S ⁱ	0.848 (16)	2.631 (16)	3.4326 (13)	158.2 (14)

Symmetry code: (i) $-x, -y + 1, -z + 1$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2003); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supporting information for this paper is available from the IUCr electronic archives (Reference: XU5831).

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supporting information

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Crystal structure of *O*-isopropyl [bis(trimethylsilyl)amino](*tert*-butylamino)-phosphinothioate

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S1. Comments

[Bis(trimethylsilyl)amino](*tert*-butylimino)thiophosphorane was first synthesized by Scherer and Kuhn in 1974, see: Scherer & Kuhn (1974), and later some general chemical reactivity of this compound was studied, see: Scherer *et al.* (1978). Based on these early results, pentavalent tricoordinated $\sigma^3\lambda^5$ -phosphoranes recommended themselves as promising ligands for the obtaining of new organometallic metallacycles with specific features. Recently we have reported and characterized series of transition metal metallacycles, containing phosphorus atom in cyclic moiety, see: Kovalenko *et al.* (2011a, 2011b, 2011c, 2012); Rusanov *et al.* (1992). In current communication we reported the reactivity of [bis(trimethylsilyl)amino](*tert*-butylimino)-thiophosphorane with isopropyl alcohol. The reaction proceeds through a 1,2-addition of $^i\text{PrO}-\text{H}$ bond across the $\text{P}=\text{N}$ bond, resulting in the title compound. Resulted product was characterized by single X-ray analysis and ^1H , ^{13}C and ^{31}P NMR spectroscopy. In these latter days it was discovered that low-coordinate phosphorus compounds are catalytically active and might be efficiently applied in catalysis, see: Zhao *et al.* (2014a, 2014b); Goldys & Dixon (2014); Samuel *et al.* (2014); Kawalec *et al.* (2012); Zhang *et al.* (2007).

Central P atom possesses distorted tetrahedral environment of four different substituents: $(\text{Me}_3\text{Si})_2\text{N}-$, $^i\text{BuNH}-$ and $^i\text{PrO}-$ groups and S atom, resulting in stereocenter on phosphorus. R and S isomers form centrosymmetric dimers due to the formation of a pair of $\text{N}-\text{H}\cdots\text{S}$ type hydrogen bonds. Geometrical parameters of *O*-isopropyl [bis(trimethylsilyl)amino](*tert*-butylamino)phosphinothioate are consistent with the values reported earlier (Rusanov *et al.*, 1992; Kovalenko *et al.*, 2011a, 2011b) for the compounds containing analogous phosphinothioates, but deprotonated and coordinated to metal centers.

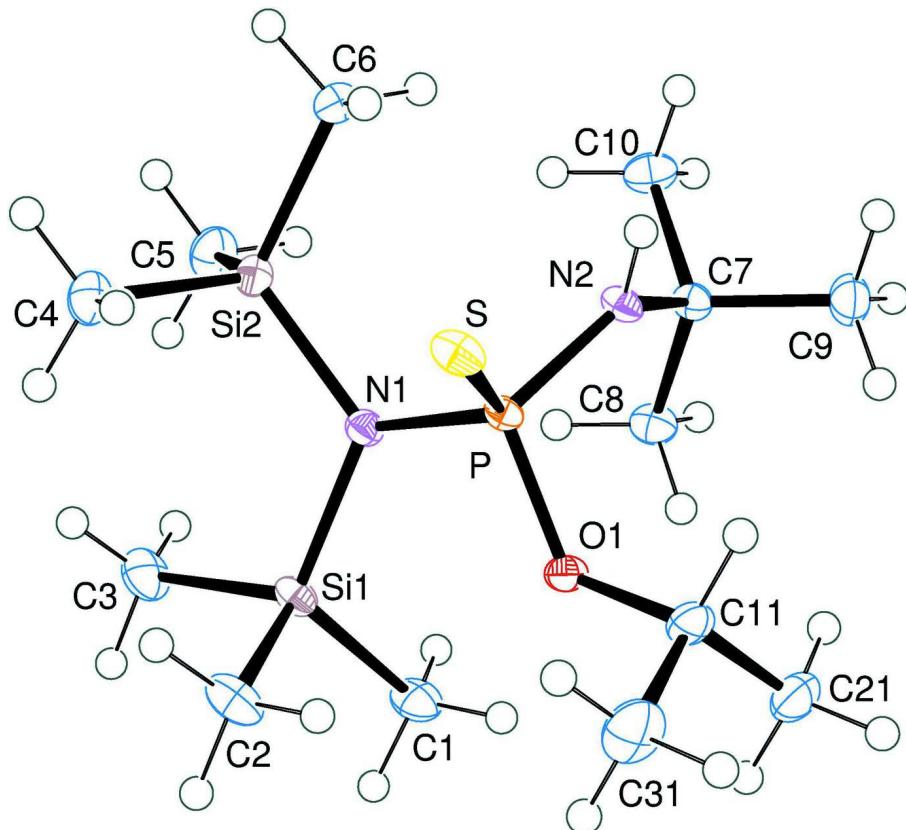
S2. Experimental

All procedures were carried out under a dry argon atmosphere using standard Schlenk and glovebox techniques. Benzene and hexane were distilled from sodium-potassium alloy directly before use. Isopropyl alcohol was dried and distilled from magnesium and stored over 4 Å molecular sieves prior to use.

In a Schlenk flask, (0.884 g, 3.0 mmol) of [bis(trimethylsilyl)amino](*tert*-butylimino)thiophosphorane was dissolved in 3 ml of benzene and the solution of isopropyl alcohol (0.23 ml, 3.0 mmol) in 1 ml of benzene was added dropwise. The mixture was stirred for 1.5 h at room temperature, thereafter solvent was removed in *vacuo* producing an almost colorless tar. The residue was dissolved in 1 ml of hexane and kept at 252 K in order to induce further crystallization. Yield: 0.76 g, 71% of colorless crystals. ^1H NMR (400 MHz, C_6D_6 , 298K): δ 5.00 (m, 1H), 2.45 (d, $^2J_{\text{P}-\text{H}}=10.3$ Hz, 1H), 1.27 (d, $^3J_{\text{H}-\text{H}}=6.0$ Hz, 3H), 1.19 (d, $^3J_{\text{H}-\text{H}}=6.0$ Hz, 3H), 1.15 (s, 9H), 0.47 (18H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , 298K): δ 71.52 (d, $^2J_{\text{P}-\text{C}}=4.6$ Hz), 52.72 (d, $^2J_{\text{P}-\text{C}}=4.6$ Hz), 31.58, 31.53, 23.98, 23.92, 5.26 (d, $^3J_{\text{P}-\text{C}}=2.3$ Hz); $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, C_6D_6 , 298K): δ 63.24 (dd, $^2J_{\text{P}-\text{H}}=10.3$ Hz, $^3J_{\text{P}-\text{H}}=10.3$ Hz).

S3. Refinement

Positions of hydrogen atoms bonded to carbon were generated in idealized geometries using a riding model with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ or $1.2U_{\text{eq}}(\text{C})$. The fractional coordinates of the H atom attached to N2 were identified from a difference Fourier map and refined freely with isotropic thermal displacement parameter.

**Figure 1**

An *ORTEP* view of the molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

O*-Isopropyl [bis(trimethylsilyl)amino](tert-butylamino)phosphinothioate*Crystal data**

$\text{C}_{13}\text{H}_{33}\text{N}_2\text{OPSSi}_2$
 $M_r = 354.64$
Monoclinic, $P2_1/n$
 $a = 9.942 (3)$ Å
 $b = 11.907 (3)$ Å
 $c = 17.726 (5)$ Å
 $\beta = 100.52 (3)^\circ$
 $V = 2063.1 (10)$ Å³
 $Z = 4$

$F(000) = 776$
 $D_x = 1.142 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25646 reflections
 $\theta = 4\text{--}32.6^\circ$
 $\mu = 0.35 \text{ mm}^{-1}$
 $T = 100$ K
Block, colourless
 $0.30 \times 0.20 \times 0.20$ mm

Data collection

Oxford Xcalibur PX κ -geometry
diffractometer with a CCD area detector
Radiation source: fine-focus sealed tube
Graphite monochromator
 ω and φ scans
36939 measured reflections
7436 independent reflections

5938 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 $\theta_{\text{max}} = 32.6^\circ$, $\theta_{\text{min}} = 4.7^\circ$
 $h = -15 \rightarrow 14$
 $k = -17 \rightarrow 18$
 $l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.115$
 $S = 1.08$
7436 reflections
184 parameters
0 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.071P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.019$
 $\Delta\rho_{\text{max}} = 0.84 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.34 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S	0.06612 (3)	0.50611 (2)	0.38496 (2)	0.01778 (8)
P	0.03058 (3)	0.34478 (2)	0.38973 (2)	0.01212 (8)
O1	-0.06932 (9)	0.29955 (7)	0.31509 (5)	0.01497 (17)
C11	-0.19850 (13)	0.35845 (11)	0.28645 (7)	0.0197 (2)
H11	-0.2199	0.4103	0.3270	0.024*
C21	-0.30994 (14)	0.27054 (13)	0.26853 (8)	0.0265 (3)
H21A	-0.3976	0.3074	0.2492	0.040*
H21B	-0.2880	0.2189	0.2295	0.040*
H21C	-0.3163	0.2285	0.3153	0.040*
C31	-0.18259 (16)	0.42557 (13)	0.21616 (9)	0.0307 (3)
H31A	-0.2682	0.4653	0.1965	0.046*
H31B	-0.1084	0.4802	0.2299	0.046*
H31C	-0.1609	0.3747	0.1766	0.046*
Si1	0.18608 (4)	0.19371 (3)	0.30180 (2)	0.01607 (8)
C1	0.05411 (14)	0.08448 (11)	0.26893 (8)	0.0228 (3)
H1A	0.0714	0.0505	0.2212	0.034*

H1B	0.0584	0.0263	0.3084	0.034*
H1C	-0.0368	0.1191	0.2598	0.034*
C2	0.19037 (16)	0.29925 (12)	0.22471 (8)	0.0257 (3)
H2A	0.2019	0.2607	0.1774	0.038*
H2B	0.1044	0.3417	0.2155	0.038*
H2C	0.2671	0.3509	0.2406	0.038*
C3	0.35141 (14)	0.11555 (12)	0.31640 (9)	0.0255 (3)
H3A	0.3617	0.0785	0.2684	0.038*
H3B	0.4272	0.1682	0.3319	0.038*
H3C	0.3521	0.0589	0.3566	0.038*
Si2	0.31243 (3)	0.29123 (3)	0.46123 (2)	0.01629 (8)
C4	0.43267 (13)	0.38055 (12)	0.41764 (8)	0.0225 (3)
H4A	0.5138	0.3973	0.4564	0.034*
H4B	0.4602	0.3403	0.3747	0.034*
H4C	0.3870	0.4508	0.3990	0.034*
C5	0.38927 (14)	0.15588 (12)	0.50201 (9)	0.0253 (3)
H5A	0.4697	0.1716	0.5415	0.038*
H5B	0.3217	0.1142	0.5248	0.038*
H5C	0.4166	0.1109	0.4610	0.038*
C6	0.27586 (13)	0.37228 (13)	0.54548 (8)	0.0232 (3)
H6A	0.3612	0.3845	0.5820	0.035*
H6B	0.2353	0.4449	0.5281	0.035*
H6C	0.2118	0.3299	0.5705	0.035*
N1	0.16513 (10)	0.26205 (8)	0.38890 (6)	0.01379 (19)
N2	-0.04109 (11)	0.31950 (8)	0.46402 (6)	0.01388 (19)
H2	-0.0419 (15)	0.3767 (13)	0.4924 (9)	0.017*
C7	-0.09601 (12)	0.21560 (10)	0.49410 (7)	0.0143 (2)
C8	-0.08932 (13)	0.11580 (10)	0.44119 (7)	0.0186 (2)
H8A	-0.1261	0.0490	0.4626	0.028*
H8B	-0.1436	0.1320	0.3904	0.028*
H8C	0.0060	0.1021	0.4365	0.028*
C9	-0.24488 (13)	0.23858 (12)	0.50102 (8)	0.0228 (3)
H9A	-0.2838	0.1715	0.5207	0.034*
H9B	-0.2482	0.3014	0.5363	0.034*
H9C	-0.2978	0.2576	0.4504	0.034*
C10	-0.01281 (14)	0.18979 (11)	0.57379 (7)	0.0204 (3)
H10A	-0.0483	0.1215	0.5940	0.031*
H10B	0.0834	0.1786	0.5700	0.031*
H10C	-0.0203	0.2528	0.6084	0.031*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.02695 (17)	0.01109 (14)	0.01685 (16)	-0.00040 (11)	0.00810 (12)	-0.00059 (10)
P	0.01485 (14)	0.01073 (14)	0.01114 (15)	0.00093 (10)	0.00329 (10)	-0.00069 (10)
O1	0.0162 (4)	0.0156 (4)	0.0123 (4)	0.0025 (3)	0.0005 (3)	-0.0018 (3)
C11	0.0177 (6)	0.0237 (6)	0.0160 (6)	0.0053 (5)	-0.0016 (4)	0.0004 (5)
C21	0.0183 (6)	0.0372 (8)	0.0216 (7)	-0.0017 (6)	-0.0022 (5)	0.0035 (6)

C31	0.0283 (7)	0.0317 (8)	0.0293 (8)	0.0040 (6)	-0.0019 (6)	0.0135 (6)
Si1	0.02069 (17)	0.01375 (16)	0.01521 (17)	0.00146 (12)	0.00709 (13)	-0.00205 (12)
C1	0.0300 (7)	0.0182 (6)	0.0211 (7)	-0.0017 (5)	0.0072 (5)	-0.0070 (5)
C2	0.0360 (8)	0.0242 (7)	0.0199 (7)	0.0012 (6)	0.0135 (6)	0.0019 (5)
C3	0.0258 (7)	0.0239 (7)	0.0290 (8)	0.0058 (5)	0.0105 (5)	-0.0047 (6)
Si2	0.01396 (16)	0.01862 (17)	0.01629 (18)	-0.00085 (12)	0.00281 (12)	0.00010 (13)
C4	0.0189 (6)	0.0226 (6)	0.0267 (7)	-0.0031 (5)	0.0058 (5)	0.0002 (5)
C5	0.0212 (6)	0.0270 (7)	0.0265 (7)	0.0028 (5)	0.0016 (5)	0.0071 (6)
C6	0.0183 (6)	0.0330 (7)	0.0174 (6)	-0.0049 (5)	0.0014 (5)	-0.0052 (5)
N1	0.0144 (4)	0.0143 (4)	0.0129 (5)	0.0012 (4)	0.0031 (3)	-0.0009 (4)
N2	0.0188 (5)	0.0115 (4)	0.0124 (5)	-0.0008 (4)	0.0058 (4)	-0.0021 (4)
C7	0.0165 (5)	0.0133 (5)	0.0133 (5)	-0.0009 (4)	0.0035 (4)	0.0011 (4)
C8	0.0245 (6)	0.0135 (5)	0.0181 (6)	-0.0029 (4)	0.0044 (5)	-0.0013 (5)
C9	0.0172 (6)	0.0255 (7)	0.0267 (7)	-0.0016 (5)	0.0065 (5)	-0.0007 (5)
C10	0.0275 (7)	0.0161 (6)	0.0158 (6)	0.0000 (5)	-0.0010 (5)	0.0023 (5)

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

S—P	1.9578 (6)	Si2—N1	1.7954 (12)
P—O1	1.5959 (10)	Si2—C6	1.8687 (14)
P—N2	1.6356 (11)	Si2—C4	1.8694 (14)
P—N1	1.6635 (11)	Si2—C5	1.8713 (14)
O1—C11	1.4700 (15)	C4—H4A	0.9800
C11—C31	1.513 (2)	C4—H4B	0.9800
C11—C21	1.515 (2)	C4—H4C	0.9800
C11—H11	1.0000	C5—H5A	0.9800
C21—H21A	0.9800	C5—H5B	0.9800
C21—H21B	0.9800	C5—H5C	0.9800
C21—H21C	0.9800	C6—H6A	0.9800
C31—H31A	0.9800	C6—H6B	0.9800
C31—H31B	0.9800	C6—H6C	0.9800
C31—H31C	0.9800	N2—C7	1.4898 (15)
Si1—N1	1.7907 (11)	N2—H2	0.848 (16)
Si1—C2	1.8628 (14)	C7—C8	1.5228 (17)
Si1—C1	1.8637 (14)	C7—C9	1.5319 (17)
Si1—C3	1.8653 (14)	C7—C10	1.5320 (18)
C1—H1A	0.9800	C8—H8A	0.9800
C1—H1B	0.9800	C8—H8B	0.9800
C1—H1C	0.9800	C8—H8C	0.9800
C2—H2A	0.9800	C9—H9A	0.9800
C2—H2B	0.9800	C9—H9B	0.9800
C2—H2C	0.9800	C9—H9C	0.9800
C3—H3A	0.9800	C10—H10A	0.9800
C3—H3B	0.9800	C10—H10B	0.9800
C3—H3C	0.9800	C10—H10C	0.9800
O1—P—N2		N1—Si2—C5	109.36 (6)
O1—P—N1		C6—Si2—C5	105.15 (7)

N2—P—N1	111.55 (6)	C4—Si2—C5	113.76 (7)
O1—P—S	112.66 (4)	Si2—C4—H4A	109.5
N2—P—S	108.90 (4)	Si2—C4—H4B	109.5
N1—P—S	115.40 (4)	H4A—C4—H4B	109.5
C11—O1—P	119.84 (8)	Si2—C4—H4C	109.5
O1—C11—C31	108.69 (11)	H4A—C4—H4C	109.5
O1—C11—C21	107.59 (11)	H4B—C4—H4C	109.5
C31—C11—C21	112.01 (12)	Si2—C5—H5A	109.5
O1—C11—H11	109.5	Si2—C5—H5B	109.5
C31—C11—H11	109.5	H5A—C5—H5B	109.5
C21—C11—H11	109.5	Si2—C5—H5C	109.5
C11—C21—H21A	109.5	H5A—C5—H5C	109.5
C11—C21—H21B	109.5	H5B—C5—H5C	109.5
H21A—C21—H21B	109.5	Si2—C6—H6A	109.5
C11—C21—H21C	109.5	Si2—C6—H6B	109.5
H21A—C21—H21C	109.5	H6A—C6—H6B	109.5
H21B—C21—H21C	109.5	Si2—C6—H6C	109.5
C11—C31—H31A	109.5	H6A—C6—H6C	109.5
C11—C31—H31B	109.5	H6B—C6—H6C	109.5
H31A—C31—H31B	109.5	P—N1—Si1	119.80 (6)
C11—C31—H31C	109.5	P—N1—Si2	115.56 (6)
H31A—C31—H31C	109.5	Si1—N1—Si2	119.70 (6)
H31B—C31—H31C	109.5	C7—N2—P	133.08 (8)
N1—Si1—C2	110.35 (6)	C7—N2—H2	114.3 (11)
N1—Si1—C1	113.62 (6)	P—N2—H2	112.5 (11)
C2—Si1—C1	110.52 (7)	N2—C7—C8	111.56 (10)
N1—Si1—C3	110.20 (6)	N2—C7—C9	107.63 (10)
C2—Si1—C3	107.50 (7)	C8—C7—C9	109.89 (11)
C1—Si1—C3	104.33 (7)	N2—C7—C10	108.97 (10)
Si1—C1—H1A	109.5	C8—C7—C10	109.54 (10)
Si1—C1—H1B	109.5	C9—C7—C10	109.20 (11)
H1A—C1—H1B	109.5	C7—C8—H8A	109.5
Si1—C1—H1C	109.5	C7—C8—H8B	109.5
H1A—C1—H1C	109.5	H8A—C8—H8B	109.5
H1B—C1—H1C	109.5	C7—C8—H8C	109.5
Si1—C2—H2A	109.5	H8A—C8—H8C	109.5
Si1—C2—H2B	109.5	H8B—C8—H8C	109.5
H2A—C2—H2B	109.5	C7—C9—H9A	109.5
Si1—C2—H2C	109.5	C7—C9—H9B	109.5
H2A—C2—H2C	109.5	H9A—C9—H9B	109.5
H2B—C2—H2C	109.5	C7—C9—H9C	109.5
Si1—C3—H3A	109.5	H9A—C9—H9C	109.5
Si1—C3—H3B	109.5	H9B—C9—H9C	109.5
H3A—C3—H3B	109.5	C7—C10—H10A	109.5
Si1—C3—H3C	109.5	C7—C10—H10B	109.5
H3A—C3—H3C	109.5	H10A—C10—H10B	109.5
H3B—C3—H3C	109.5	C7—C10—H10C	109.5
N1—Si2—C6	114.73 (6)	H10A—C10—H10C	109.5

N1—Si2—C4	108.34 (6)	H10B—C10—H10C	109.5
C6—Si2—C4	105.60 (7)		

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···S ⁱ	0.848 (16)	2.631 (16)	3.4326 (13)	158.2 (14)

Symmetry code: (i) $-x, -y+1, -z+1$.