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Bis(*tert*-butyldimethylsilyl)(2,6-diisopropylphenyl)phosphane: the first structure of an organophosphane with two *tert*-butyldimethylsilyl (TBDMS) substituents

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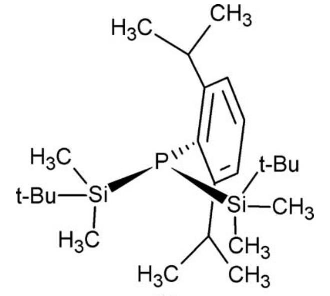
The title compound, $C_{24}H_{47}PSi_2$, is the first organophosphane bearing two *tert*-butyldimethylsilyl (TBDMS) groups to be crystallographically characterized, even though TBDMS is a very popular bulky silyl group. The structure is a considerably flattened trigonal pyramid, with the sum of the C/Si—P—C/Si angles being 333.35 (6)°, which can be attributed to the steric pressure from the three bulky groups. The P—Si distances [2.2605 (6) and 2.2631 (6) Å] are normal, while the P—C distance [1.8646 (12) Å] is long (outside the s.u. values) compared with related structures. The plane of the aryl ring approximately bisects the Si—P—Si angle, quite unlike the secondary (*tert*-butyldimethylsilyl)(2,6-diisopropylphenyl)phosphane bearing only one TBDMS group, in which the single Si atom is perpendicular to the aryl ring. The title structure conforms closely to that predicted from B3LYP/6-31G(d) calculations, although the calculations overestimate the degree of planarity. The compound crystallizes centrosymmetrically in the space group $P\overline{1}$ as isolated molecules.

Comment

The title compound, (I), was prepared as part of a larger study of functional derivatives of (2,6-diisopropylphenyl)phosphane, $DippPH_2$ (Boeré & Masuda, 2002), including the mono- and bis(trimethylsilyl)- and the mono- and bis(*tert*-butyldimethylsilyl)- (TBDMS) derivatives. The structure obtained from the diffraction study of (I), $DippP(TBDMS)_2$, can be compared with the previously published B3LYP/6-31G(d) hybrid density functional theory (DFT) calculations (Boeré & Masuda, 2002).

A key feature of phosphanes with bulky substituents is the sum of the angles about the central P atom (Boeré & Zhang, 2005). Experimentally, Σ(C,Si—P—C,Si) = 333.35 (6)° for (I), while the computed value is 346.1°. Key bond lengths are P—Si [2.2605 (6) and 2.2631 (6) Å, compared with computed values of 2.276 and 2.296 Å] and P—C [1.8646 (12) Å, compared with a computed value of 1.881 Å]. In each of these parameters, the DFT calculations overestimate, though the effect for the bond distances is small (0.7–1.45%). However, the bond-angle sum is considerably overestimated, by 3.8%. Comparisons can also be made with DippP(H)TBDMS (Boeré & Masuda, 2002) and $P(TBDMS)_3$ (Nieger *et al.*, 1997) [Cambridge Structural Database (CSD; Allen, 2002) refcodes LUTDEJ and GATROI, respectively]. In the former, the P—Si bond length is 2.2681 (9) Å, marginally longer than in (I) by 0.001–0.003 Å outside the s.u. value, while the P—C bond length is 1.854 (2) Å, shorter than in (I) by 0.005 Å outside the s.u. value. LUTDEJ, with an H atom in place of one bulky group, is of course much more pyramidal than (I). In the Nieger *et al.* structure, the average P—Si distance is 2.268 (1) Å, marginally longer than in (I). With three bulky TBDMS groups, the sums of angles can be meaningfully contrasted; thus, Σ(Si—P—Si) = 329.86 (7)°, about 1% smaller than in (I). All three TBDMS groups orient their *tert*-butyl groups *exo* to the PSi_3 pyramid, which allows for less steric congestion in the inner 'pocket', whereas in (I) only one *tert*-butyl group has this orientation, due to the greater congestion from the two flanking isopropyl groups of the Dipp ring. The P—C bond in (I) is also long by 0.009 Å outside the s.u. value compared to 1.8507 (16) Å found in the comparably



(I)

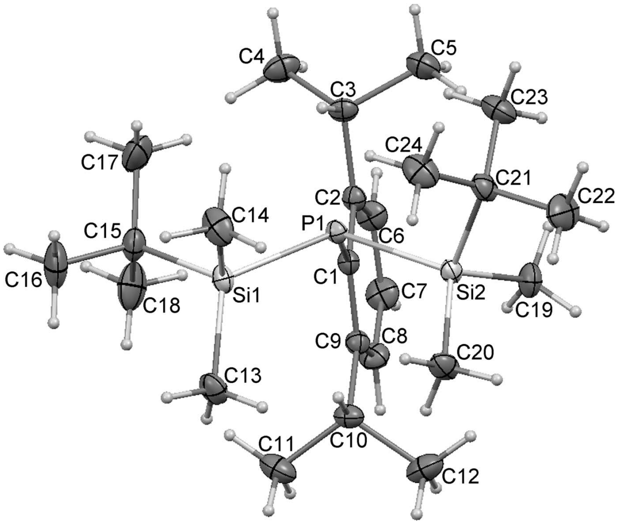


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

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congested $PDipp_3$, which has $\Sigma(C—P—C) = 335.64\ (6)^\circ$ (refcode PIXDEG; Boeré *et al.* 2008).

The TBDMS group has also been used to stabilize two compounds with P—P bonds, namely $(TBDMS)_2P—P(TBDMS)_2$ (refcode WIHJOM; Westermann & Nieger, 1990) and $(TBDMS)_2P—P(N^iPr_2)_2$ (refcode SIYXUT; Bender *et al.*, 1994). These two structures represent the only other known crystal structures with TBDMS groups attached to P, despite the widespread use of this popular bulky hydride synthon in preparative phosphorus chemistry.

Just three crystal structures of phosphanes bearing one aryl and two trimethylsilyl groups have been reported in the literature [refcodes GEDDAU (Cowley *et al.*, 1987), and SIQBEZ and SIQBID (McMurran *et al.*, 1998)], but only that reported by Cowley *et al.* incorporates a bulky aryl group. In this structure, namely bis(trimethylsilyl)(2,4,6-tri-*tert*-butylphenyl)phosphane, the value for $\Sigma(C,Si—P—C,Si)$ is $343.1\ (6)^\circ$, making it the most sterically congested $PCSi_2$-substituted phosphane on record, as is also reflected in the severe structural distortion, such that the P atom in this structure is some 0.90 Å above the mean plane of the six aromatic ring C atoms (Cowley *et al.*, 1987). By contrast, in (I) the P atom is located only 0.192 (2) Å above the mean ring plane.

Experimental

Full synthetic details for the preparation of the title compound have already been published (Boeré & Masuda, 2002). At the time of the original study, crystals of (*tert*-butyldimethylsilyl)(2,6-diisopropylphenyl)phosphane, DippP(H)TBDMS, were obtained, but $DippP(TBDMS)_2$ could only be obtained as an oil or a white sublimate. Over time, while being stored at 263 K, the oil formed single crystals suitable for an X-ray diffraction study, the results of which are presented here.

Crystal data

$C_{24}H_{47}PSi_2$
$M_r = 422.77$
Triclinic, $P\bar{1}$
$a = 10.432\ (3)$ Å
$b = 11.237\ (3)$ Å
$c = 11.885\ (3)$ Å
$\alpha = 80.084\ (2)^\circ$
$\beta = 88.989\ (2)^\circ$
$\gamma = 88.943\ (2)^\circ$
$V = 1372.0\ (6)$ Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.20$ mm^{-1}
$T = 173$ K
0.49 × 0.32 × 0.24 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{\min} = 0.708$, $T_{\max} = 0.746$
16018 measured reflections
6218 independent reflections
5511 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.013$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.089$
$S = 1.04$
6218 reflections
258 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.33$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}

C-bound H atoms were treated as riding, with C—H = 0.98 Å and $U_{\rm iso}(H) = 1.5U_{\rm eq}(C)$ for methyl, C—H = 1.00 Å and $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$ for methine, and C—H = 0.95 Å and $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$ for aromatic H atoms. No data were rejected and the largest peak and hole in the final difference map were much smaller than the equivalent electron density of an H atom.

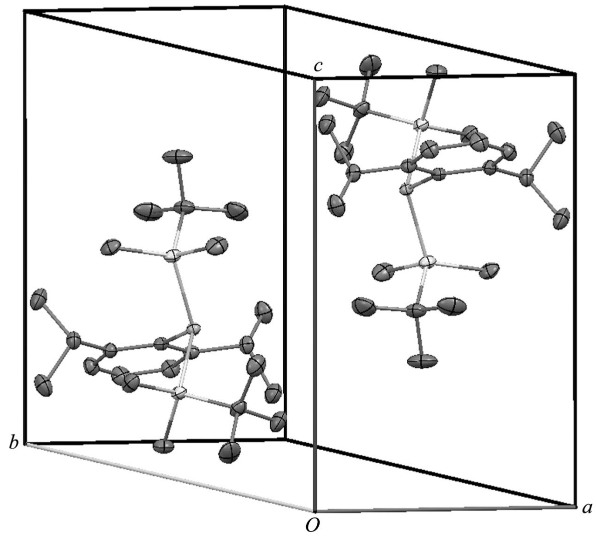

Figure 2
A crystal packing diagram for (I), showing the centrosymmetric arrangement of the two $PCSi_2$ pyramids within the unit cell.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT-Plus* (Bruker, 2008); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK3445). Services for accessing these data are described at the back of the journal.

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supplementary materials

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$\gamma = 88.943\ (2)°$
$V = 1372.0\ (6)$ Å^3

$Z = 2$
$F(000) = 468$
$D_x = 1.023$ Mg m^{-3}
Melting point: 330 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9974 reflections
$\theta = 2.3–27.5°$
$\mu = 0.20$ mm^{-1}
$T = 173$ K
Block, colourless
0.49 × 0.32 × 0.24 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube, Bruker D8
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{\min} = 0.708$, $T_{\max} = 0.746$

16018 measured reflections
6218 independent reflections
5511 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.013$
$\theta_{\max} = 27.5°$, $\theta_{\min} = 1.7°$
$h = -13 \rightarrow 13$
$k = -14 \rightarrow 14$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.089$
$S = 1.04$
6218 reflections
258 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.3449P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.33$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}

Special details

Experimental. A crystal coated in Paratone (TM) oil was mounted on the end of a thin glass capillary and cooled in the gas stream of the diffractometer Kryoflex device.

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 (Å²)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
P1	0.31838 (3)	0.70473 (2)	0.30839 (2)	0.02343 (8)
Si1	0.21935 (3)	0.68723 (3)	0.48103 (3)	0.03059 (9)
Si2	0.19876 (3)	0.64740 (3)	0.17054 (3)	0.02741 (9)
C1	0.36898 (10)	0.86155 (10)	0.24881 (9)	0.0246 (2)
C2	0.50223 (11)	0.87712 (10)	0.22579 (10)	0.0288 (2)
C3	0.60280 (11)	0.77692 (11)	0.25732 (11)	0.0336 (3)
H3	0.5597	0.7080	0.3073	0.040*
C4	0.71306 (14)	0.81667 (14)	0.32510 (15)	0.0500 (4)
H4A	0.7711	0.7478	0.3493	0.075*
H4B	0.6784	0.8462	0.3925	0.075*
H4C	0.7603	0.8814	0.2768	0.075*
C5	0.65361 (15)	0.73079 (15)	0.15145 (14)	0.0529 (4)
H5A	0.6963	0.7965	0.1004	0.079*
H5B	0.5821	0.7018	0.1116	0.079*
H5C	0.7151	0.6644	0.1743	0.079*
C6	0.54632 (13)	0.98873 (12)	0.17013 (12)	0.0387 (3)
H6	0.6353	0.9986	0.1534	0.046*
C7	0.46296 (14)	1.08497 (12)	0.13894 (12)	0.0433 (3)
H7	0.4941	1.1601	0.1001	0.052*
C8	0.33437 (13)	1.07138 (11)	0.16454 (12)	0.0383 (3)
H8	0.2779	1.1387	0.1446	0.046*
C9	0.28435 (11)	0.96182 (10)	0.21885 (10)	0.0296 (2)
C10	0.14061 (12)	0.95863 (11)	0.24407 (11)	0.0353 (3)
H10	0.1185	0.8747	0.2813	0.042*
C11	0.10247 (16)	1.04456 (14)	0.32630 (15)	0.0522 (4)
H11A	0.1572	1.0287	0.3935	0.078*
H11B	0.0127	1.0317	0.3502	0.078*
H11C	0.1131	1.1283	0.2878	0.078*
C12	0.06085 (15)	0.99134 (16)	0.13565 (15)	0.0552 (4)
H12A	0.0804	1.0738	0.0981	0.083*
H12B	−0.0306	0.9863	0.1560	0.083*
H12C	0.0817	0.9348	0.0835	0.083*
C13	0.05423 (13)	0.75282 (14)	0.49213 (12)	0.0438 (3)
H13A	−0.0003	0.7283	0.4341	0.066*
H13B	0.0586	0.8412	0.4799	0.066*

H13C	0.0179	0.7233	0.5682	0.066*
C14	0.20319 (18)	0.52051 (13)	0.52999 (13)	0.0530 (4)
H14A	0.1745	0.5050	0.6101	0.079*
H14B	0.2864	0.4803	0.5227	0.079*
H14C	0.1402	0.4890	0.4828	0.079*
C15	0.33081 (14)	0.74735 (14)	0.58242 (11)	0.0448 (3)
C16	0.2743 (2)	0.7195 (2)	0.70417 (13)	0.0727 (6)
H16A	0.2686	0.6318	0.7282	0.109*
H16B	0.1884	0.7562	0.7055	0.109*
H16C	0.3297	0.7527	0.7565	0.109*
C17	0.46314 (18)	0.6870 (2)	0.58157 (16)	0.0769 (6)
H17A	0.5186	0.7177	0.6355	0.115*
H17B	0.5009	0.7051	0.5046	0.115*
H17C	0.4549	0.5993	0.6041	0.115*
C18	0.3459 (2)	0.88479 (17)	0.55046 (16)	0.0696 (5)
H18A	0.2622	0.9247	0.5553	0.104*
H18B	0.3802	0.9049	0.4723	0.104*
H18C	0.4050	0.9125	0.6034	0.104*
C19	0.24653 (15)	0.74435 (14)	0.03199 (11)	0.0449 (3)
H19A	0.1814	0.7396	−0.0254	0.067*
H19B	0.3293	0.7158	0.0058	0.067*
H19C	0.2538	0.8283	0.0432	0.067*
C20	0.02092 (12)	0.65450 (14)	0.19423 (13)	0.0430 (3)
H20A	−0.0051	0.7371	0.2016	0.065*
H20B	−0.0025	0.5991	0.2643	0.065*
H20C	−0.0226	0.6310	0.1292	0.065*
C21	0.24529 (13)	0.48471 (12)	0.15967 (12)	0.0381 (3)
C22	0.1663 (2)	0.44403 (17)	0.06560 (17)	0.0691 (5)
H22A	0.1954	0.3633	0.0547	0.104*
H22B	0.1778	0.5011	−0.0060	0.104*
H22C	0.0755	0.4417	0.0880	0.104*
C23	0.38752 (15)	0.47457 (15)	0.12971 (15)	0.0538 (4)
H23A	0.4388	0.5015	0.1887	0.081*
H23B	0.4054	0.5254	0.0557	0.081*
H23C	0.4097	0.3903	0.1255	0.081*
C24	0.21907 (17)	0.39973 (13)	0.27232 (15)	0.0535 (4)
H24A	0.2449	0.3172	0.2647	0.080*
H24B	0.1273	0.4021	0.2912	0.080*
H24C	0.2682	0.4254	0.3332	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.02309 (14)	0.02461 (14)	0.02256 (14)	−0.00225 (10)	0.00176 (10)	−0.00397 (10)
Si1	0.03540 (18)	0.03276 (17)	0.02373 (16)	−0.00538 (13)	0.00525 (13)	−0.00523 (12)
Si2	0.02483 (15)	0.03361 (17)	0.02542 (16)	−0.00200 (12)	0.00153 (12)	−0.00970 (12)
C1	0.0275 (5)	0.0246 (5)	0.0220 (5)	−0.0027 (4)	0.0006 (4)	−0.0044 (4)
C2	0.0281 (5)	0.0309 (6)	0.0274 (5)	−0.0037 (4)	0.0018 (4)	−0.0048 (4)
C3	0.0231 (5)	0.0357 (6)	0.0412 (7)	−0.0019 (5)	0.0015 (5)	−0.0048 (5)
C4	0.0338 (7)	0.0510 (8)	0.0646 (10)	−0.0021 (6)	−0.0125 (7)	−0.0069 (7)

C5	0.0428 (8)	0.0603 (10)	0.0575 (9)	0.0104 (7)	0.0062 (7)	−0.0174 (8)
C6	0.0332 (6)	0.0385 (7)	0.0426 (7)	−0.0103 (5)	0.0059 (5)	−0.0011 (5)
C7	0.0487 (8)	0.0313 (6)	0.0462 (8)	−0.0104 (6)	0.0045 (6)	0.0040 (5)
C8	0.0443 (7)	0.0272 (6)	0.0411 (7)	0.0020 (5)	−0.0013 (6)	0.0003 (5)
C9	0.0320 (6)	0.0295 (6)	0.0272 (6)	−0.0003 (5)	−0.0004 (4)	−0.0047 (4)
C10	0.0304 (6)	0.0317 (6)	0.0423 (7)	0.0054 (5)	0.0012 (5)	−0.0029 (5)
C11	0.0511 (9)	0.0414 (8)	0.0646 (10)	0.0080 (6)	0.0159 (7)	−0.0133 (7)
C12	0.0405 (8)	0.0584 (10)	0.0625 (10)	0.0079 (7)	−0.0129 (7)	0.0016 (8)
C13	0.0373 (7)	0.0549 (8)	0.0403 (7)	−0.0052 (6)	0.0140 (6)	−0.0124 (6)
C14	0.0736 (11)	0.0383 (7)	0.0439 (8)	−0.0106 (7)	0.0202 (7)	0.0007 (6)
C15	0.0493 (8)	0.0598 (9)	0.0269 (6)	−0.0066 (7)	−0.0031 (6)	−0.0108 (6)
C16	0.0905 (14)	0.1034 (15)	0.0277 (8)	−0.0224 (12)	0.0031 (8)	−0.0192 (9)
C17	0.0578 (11)	0.1255 (19)	0.0515 (10)	0.0109 (11)	−0.0231 (8)	−0.0263 (11)
C18	0.0967 (15)	0.0670 (11)	0.0504 (10)	−0.0316 (10)	−0.0149 (9)	−0.0204 (8)
C19	0.0547 (8)	0.0533 (8)	0.0263 (6)	−0.0039 (7)	0.0014 (6)	−0.0049 (6)
C20	0.0260 (6)	0.0561 (8)	0.0524 (8)	−0.0029 (6)	−0.0012 (5)	−0.0245 (7)
C21	0.0398 (7)	0.0382 (7)	0.0410 (7)	−0.0008 (5)	0.0006 (5)	−0.0197 (6)
C22	0.0797 (13)	0.0630 (11)	0.0774 (13)	0.0094 (9)	−0.0254 (10)	−0.0466 (10)
C23	0.0493 (9)	0.0527 (9)	0.0619 (10)	0.0122 (7)	0.0129 (7)	−0.0192 (8)
C24	0.0638 (10)	0.0330 (7)	0.0641 (10)	−0.0058 (7)	0.0105 (8)	−0.0102 (7)

Geometric parameters (Å, º)

P1—C1	1.8646 (12)	C12—H12C	0.9800
P1—Si1	2.2605 (6)	C13—H13A	0.9800
P1—Si2	2.2631 (5)	C13—H13B	0.9800
Si1—C13	1.8725 (15)	C13—H13C	0.9800
Si1—C14	1.8734 (15)	C14—H14A	0.9800
Si1—C15	1.9024 (14)	C14—H14B	0.9800
Si2—C20	1.8738 (14)	C14—H14C	0.9800
Si2—C19	1.8761 (14)	C15—C17	1.528 (2)
Si2—C21	1.9080 (14)	C15—C18	1.536 (2)
C1—C9	1.4185 (16)	C15—C16	1.536 (2)
C1—C2	1.4201 (16)	C16—H16A	0.9800
C2—C6	1.3953 (17)	C16—H16B	0.9800
C2—C3	1.5277 (17)	C16—H16C	0.9800
C3—C5	1.524 (2)	C17—H17A	0.9800
C3—C4	1.5320 (18)	C17—H17B	0.9800
C3—H3	1.0000	C17—H17C	0.9800
C4—H4A	0.9800	C18—H18A	0.9800
C4—H4B	0.9800	C18—H18B	0.9800
C4—H4C	0.9800	C18—H18C	0.9800
C5—H5A	0.9800	C19—H19A	0.9800
C5—H5B	0.9800	C19—H19B	0.9800
C5—H5C	0.9800	C19—H19C	0.9800
C6—C7	1.379 (2)	C20—H20A	0.9800
C6—H6	0.9500	C20—H20B	0.9800
C7—C8	1.376 (2)	C20—H20C	0.9800
C7—H7	0.9500	C21—C23	1.527 (2)
C8—C9	1.3938 (17)	C21—C24	1.528 (2)

C8—H8	0.9500	C21—C22	1.536 (2)
C9—C10	1.5238 (17)	C22—H22A	0.9800
C10—C11	1.5307 (19)	C22—H22B	0.9800
C10—C12	1.533 (2)	C22—H22C	0.9800
C10—H10	1.0000	C23—H23A	0.9800
C11—H11A	0.9800	C23—H23B	0.9800
C11—H11B	0.9800	C23—H23C	0.9800
C11—H11C	0.9800	C24—H24A	0.9800
C12—H12A	0.9800	C24—H24B	0.9800
C12—H12B	0.9800	C24—H24C	0.9800

C1—P1—Si1	113.81 (4)	H13A—C13—H13B	109.5
C1—P1—Si2	105.10 (4)	Si1—C13—H13C	109.5
Si1—P1—Si2	114.44 (2)	H13A—C13—H13C	109.5
C13—Si1—C14	105.60 (7)	H13B—C13—H13C	109.5
C13—Si1—C15	109.98 (7)	Si1—C14—H14A	109.5
C14—Si1—C15	108.24 (8)	Si1—C14—H14B	109.5
C13—Si1—P1	119.57 (5)	H14A—C14—H14B	109.5
C14—Si1—P1	104.70 (5)	Si1—C14—H14C	109.5
C15—Si1—P1	108.15 (5)	H14A—C14—H14C	109.5
C20—Si2—C19	110.85 (7)	H14B—C14—H14C	109.5
C20—Si2—C21	107.97 (6)	C17—C15—C18	108.82 (16)
C19—Si2—C21	107.31 (7)	C17—C15—C16	108.64 (14)
C20—Si2—P1	115.36 (5)	C18—C15—C16	108.04 (14)
C19—Si2—P1	106.98 (5)	C17—C15—Si1	110.64 (11)
C21—Si2—P1	108.06 (4)	C18—C15—Si1	111.60 (10)
C9—C1—C2	118.94 (10)	C16—C15—Si1	109.01 (11)
C9—C1—P1	124.98 (9)	C15—C16—H16A	109.5
C2—C1—P1	115.95 (8)	C15—C16—H16B	109.5
C6—C2—C1	119.51 (11)	H16A—C16—H16B	109.5
C6—C2—C3	116.85 (11)	C15—C16—H16C	109.5
C1—C2—C3	123.64 (10)	H16A—C16—H16C	109.5
C5—C3—C2	111.09 (11)	H16B—C16—H16C	109.5
C5—C3—C4	110.79 (12)	C15—C17—H17A	109.5
C2—C3—C4	112.24 (11)	C15—C17—H17B	109.5
C5—C3—H3	107.5	H17A—C17—H17B	109.5
C2—C3—H3	107.5	C15—C17—H17C	109.5
C4—C3—H3	107.5	H17A—C17—H17C	109.5
C3—C4—H4A	109.5	H17B—C17—H17C	109.5
C3—C4—H4B	109.5	C15—C18—H18A	109.5
H4A—C4—H4B	109.5	C15—C18—H18B	109.5
C3—C4—H4C	109.5	H18A—C18—H18B	109.5
H4A—C4—H4C	109.5	C15—C18—H18C	109.5
H4B—C4—H4C	109.5	H18A—C18—H18C	109.5
C3—C5—H5A	109.5	H18B—C18—H18C	109.5
C3—C5—H5B	109.5	Si2—C19—H19A	109.5
H5A—C5—H5B	109.5	Si2—C19—H19B	109.5
C3—C5—H5C	109.5	H19A—C19—H19B	109.5
H5A—C5—H5C	109.5	Si2—C19—H19C	109.5

H5B—C5—H5C	109.5	H19A—C19—H19C	109.5
C7—C6—C2	121.13 (12)	H19B—C19—H19C	109.5
C7—C6—H6	119.4	Si2—C20—H20A	109.5
C2—C6—H6	119.4	Si2—C20—H20B	109.5
C8—C7—C6	119.52 (12)	H20A—C20—H20B	109.5
C8—C7—H7	120.2	Si2—C20—H20C	109.5
C6—C7—H7	120.2	H20A—C20—H20C	109.5
C7—C8—C9	122.02 (12)	H20B—C20—H20C	109.5
C7—C8—H8	119.0	C23—C21—C24	108.24 (13)
C9—C8—H8	119.0	C23—C21—C22	108.82 (13)
C8—C9—C1	118.83 (11)	C24—C21—C22	108.73 (13)
C8—C9—C10	117.08 (11)	C23—C21—Si2	110.75 (10)
C1—C9—C10	124.08 (10)	C24—C21—Si2	111.16 (9)
C9—C10—C11	111.23 (11)	C22—C21—Si2	109.09 (10)
C9—C10—C12	112.53 (11)	C21—C22—H22A	109.5
C11—C10—C12	108.60 (12)	C21—C22—H22B	109.5
C9—C10—H10	108.1	H22A—C22—H22B	109.5
C11—C10—H10	108.1	C21—C22—H22C	109.5
C12—C10—H10	108.1	H22A—C22—H22C	109.5
C10—C11—H11A	109.5	H22B—C22—H22C	109.5
C10—C11—H11B	109.5	C21—C23—H23A	109.5
H11A—C11—H11B	109.5	C21—C23—H23B	109.5
C10—C11—H11C	109.5	H23A—C23—H23B	109.5
H11A—C11—H11C	109.5	C21—C23—H23C	109.5
H11B—C11—H11C	109.5	H23A—C23—H23C	109.5
C10—C12—H12A	109.5	H23B—C23—H23C	109.5
C10—C12—H12B	109.5	C21—C24—H24A	109.5
H12A—C12—H12B	109.5	C21—C24—H24B	109.5
C10—C12—H12C	109.5	H24A—C24—H24B	109.5
H12A—C12—H12C	109.5	C21—C24—H24C	109.5
H12B—C12—H12C	109.5	H24A—C24—H24C	109.5
Si1—C13—H13A	109.5	H24B—C24—H24C	109.5
Si1—C13—H13B	109.5		

C1—P1—Si1—C13	70.76 (7)	C7—C8—C9—C1	0.2 (2)
Si2—P1—Si1—C13	−50.12 (6)	C7—C8—C9—C10	179.18 (13)
C1—P1—Si1—C14	−171.31 (7)	C2—C1—C9—C8	1.98 (17)
Si2—P1—Si1—C14	67.81 (6)	P1—C1—C9—C8	−173.63 (9)
C1—P1—Si1—C15	−56.07 (7)	C2—C1—C9—C10	−176.94 (11)
Si2—P1—Si1—C15	−176.94 (5)	P1—C1—C9—C10	7.45 (16)
C1—P1—Si2—C20	−101.47 (7)	C8—C9—C10—C11	−62.57 (15)
Si1—P1—Si2—C20	24.11 (6)	C1—C9—C10—C11	116.37 (13)
C1—P1—Si2—C19	22.35 (6)	C8—C9—C10—C12	59.54 (16)
Si1—P1—Si2—C19	147.93 (5)	C1—C9—C10—C12	−121.53 (13)
C1—P1—Si2—C21	137.61 (6)	C13—Si1—C15—C17	175.41 (12)
Si1—P1—Si2—C21	−96.80 (5)	C14—Si1—C15—C17	60.51 (14)
Si1—P1—C1—C9	−63.61 (10)	P1—Si1—C15—C17	−52.40 (13)
Si2—P1—C1—C9	62.36 (10)	C13—Si1—C15—C18	−63.26 (14)
Si1—P1—C1—C2	120.66 (8)	C14—Si1—C15—C18	−178.16 (12)

Si2—P1—C1—C2	−113.36 (8)	P1—Si1—C15—C18	68.93 (13)
C9—C1—C2—C6	−2.67 (17)	C13—Si1—C15—C16	56.00 (14)
P1—C1—C2—C6	173.33 (9)	C14—Si1—C15—C16	−58.90 (14)
C9—C1—C2—C3	178.15 (11)	P1—Si1—C15—C16	−171.81 (12)
P1—C1—C2—C3	−5.86 (15)	C20—Si2—C21—C23	174.95 (10)
C6—C2—C3—C5	−71.89 (15)	C19—Si2—C21—C23	55.41 (12)
C1—C2—C3—C5	107.31 (14)	P1—Si2—C21—C23	−59.64 (11)
C6—C2—C3—C4	52.76 (16)	C20—Si2—C21—C24	−64.68 (12)
C1—C2—C3—C4	−128.04 (13)	C19—Si2—C21—C24	175.78 (10)
C1—C2—C6—C7	1.2 (2)	P1—Si2—C21—C24	60.73 (11)
C3—C2—C6—C7	−179.54 (12)	C20—Si2—C21—C22	55.21 (13)
C2—C6—C7—C8	1.0 (2)	C19—Si2—C21—C22	−64.33 (13)
C6—C7—C8—C9	−1.7 (2)	P1—Si2—C21—C22	−179.38 (11)