

Supplementary Information

Experimental

All reactions were carried out under an argon atmosphere or in a sealed tube. Trichlorosilane and 1-butene (Tokyo Kasei co. ltd.) were purified by vacuum distillation. Chiral ligands, (*S*)- and (*R*)- 2-diphenylphosphino-2'-methoxy-1,1'-binaphtyl (MOP)¹ were synthesized by reported procedure. Allylpalladium(II) chloride dimer (Tokyo Kasei co. ltd.) was used as received. Phenylmagnesium chloride solution was prepared from chlorobenzene and magnesium in THF by standard procedure.

GLC measurements were recorded with a Shimadzu GC-8A using 10% KF-96 on celite-545 packed column. Preparative HPLC separation was carried out on a JAI LC-908 with octadecyl-silanized column with MeOH as an eluent. Nuclear magnetic resonance spectra were obtained by JEOL α -500 (¹H at 500 MHz, ¹³C at 126 MHz, and ²⁹Si at 99 MHz) with Me₄Si as an external standard. Mass spectra were recorded with JEOL JMS-700 by GLC or direct-inlet method. IR spectra were recorded with a Shimadzu FTIR-8700. Circular dichroism spectrometry was performed on a JASCO J720W CD spectrophotometer.

Synthesis of dichloro-(*S*)-2-butylphenylsilane

In a 500 ml Pyrex-glass sealed tube, (*R*)- 2-diphenylphosphino-2'-methoxy-1,1'-binaphtyl (4.19 g, 8.94 mmol), allylpalladium(II) chloride dimer (1.60 g, 4.38 mmol), and dehydrated benzene (15 ml) was placed. The tube was cooled, and 1-butene (100 g 1.79 mol) and trichlorosilane (250 g, 1.85 mol) were vacuum-transferred. The Pyrex tube was sealed and heated to 35°C for 7 days. The tube was opened and concentrated under reduced pressure. Rough distillation of the mixture gave a mixture of trichloro-1-butyldisilane and trichloro-(*S*)-2-butyldisilane as colorless liquid (267 g, 78%). A solution of PhMgCl in dry THF (1.4 mol) was added dropwise to a solution of the mixture of trichloro-1-butyldisilane and trichloro-(*S*)-2-butyldisilane (232 g, 1.21 mol) in THF (800 ml) for 3 hours. The mixture was refluxed for 1 day. The mixture was filtered and concentrated. Distillation under reduced pressure gave pure dichloro-(*S*)-2-butylphenylsilane as a colorless liquid (163 g, 58%)

¹H NMR (500MHz, CDCl₃) δ 0.84 (t, 3H, *J* = 7.4 Hz), 1.05-1.32 (m, 5H), 1.72-1.80 (m, 1H), 7.14-7.30 (m, 3H), 7.70-7.74 (m, 2H). ¹³C NMR (128 MHz, CDCl₃) δ 12.4, 12.8, 23.4, 26.5, 128.5, 131.6, 134.1. IR (neat, cm⁻¹) 2963, 2932, 2874, 2359, 2341, 1591, 1460, 1381, 1115, 1091, 999, 851, 739, 567, 517.

¹ Y. Uozumi, A. Tanahashi, S. Y. Lee, and T. Hayashi, J. Org. Chem., 58(7), 1945-1948 (1993).

Synthesis of 2,4,6-tri((*S*)-2-butyl)-2,4,6-triphenylcyclotrisiloxane (*S*)-**3**.

Aqueous NaOH solution (10 ml, 2.5 mol/l) was added to a solution of dichloro-(*S*)-2-butylphenylsilane (2.96 g, 13.0 mmol) in THF (10 ml) and benzene (10 ml). The solution was refluxed for 12 h. The mixture was washed three times with water and was concentrated. The mixture was separated with recycle-type HPLC to *cis,cis*-2,4,6-tri((*S*)-2-butyl)-2,4,6-triphenylcyclotrisiloxane (*cis,cis*-(*S*)-**3**) (120 mg, 5%) and *cis,trans*-2,4,6-tri((*S*)-2-butyl)-2,4,6-triphenylcyclotrisiloxane (*cis,trans*-(*S*)-**3**) (630 mg, 28%).

cis,cis-(*S*)-**3**: colorless liquid. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 0.99 (t, 9H, $J = 7.5$ Hz), 1.03-1.07 (m, 3H), 1.11 (d, 9H, $J = 7.1$ Hz), 1.24-1.30 (m, 3H), 1.69-1.74 (m, 3H), 7.13 (t, 6H, $J = 7.9$ Hz). $^{13}\text{C NMR}$ (128 MHz, CDCl_3) δ 12.9, 13.4, 22.7, 23.8, 127.2, 129.5, 133.8, 134.4. $^{29}\text{Si NMR}$ (99 MHz, CDCl_3) δ -26.17. MS (EI, 70 eV) m/z (%) 534 (M^+ , 4), 477 (100). IR (neat, cm^{-1}) 3071, 2959, 2930, 2870, 2856, 1958, 1884, 1591, 1460, 1429, 1379, 1215, 1123, 1033, 1013, 993, 854, 733, 696, 598, 513.

cis,trans-(*S*)-**3**: colorless waxy semisolid. $^1\text{H NMR}$ (500 MHz, CDCl_3) 0.69-0.78 (m, 7H), 0.88 (t, 8H, $J = 6.9$ Hz), 0.91-0.99 (m, 7H), 1.12-1.17 (m, 3H), 1.37-1.50 (m, 1H), 1.57-1.62 (m, 3H), 7.29-7.43 (m, 10H), 7.59-7.63 (m, 3H), 7.71-7.74 (m, 2H). $^{13}\text{C NMR}$ (128 MHz, CDCl_3) δ 12.55, 12.76, 12.82, 13.09, 13.26, 13.29, 22.45, 22.61, 22.70, 23.45, 23.67, 23.83, 127.4, 127.6, 129.7, 129.8, 133.8, 133.9, 134.8, 135.1, $^{29}\text{Si NMR}$ (99 MHz, CDCl_3) δ -23.28, -23.27, -23.05. MS (EI, 70 eV) m/z (%) 534 (M^+ , 1), 477 (98), 421 (70), 365 (100). IR (neat, cm^{-1}) 3071, 2959, 2870, 1958, 1884, 1460, 1429, 1122, 1034, 993, 733, 696.

Synthesis of (*S*)-**1** from dimethylsulfoxide and dichlorosilane.

An toluene solution (20 ml) of dehydrated dimethylsulfoxide (3.12 g, 40.0 mmol) was added dichloro-(*S*)-2-butylphenylsilane (4.66 g, 20.0 mmol) and was refluxed for 24 h. The mixture was washed three times with water and concentrated. The resulted residue was distilled by Kugelrohr apparatus (300°C/40 Pa) to gave oily mixture of *cis,cis*-(*S*)-**1** and *cis,trans*-(*S*)-**1** (2.60 g 73%). The isomeric content was checked by $^1\text{H NMR}$ measurement (16.4 : 83.6).

Crystallographic analysis of hexaphenylcyclotrisiloxane *P*-**4**

Data Collection

A colorless prismatic crystal of $\text{C}_{36}\text{H}_{30}\text{Si}_3\text{O}_3$ having approximate dimensions of 0.60 x 0.60 x 0.50 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC7S diffractometer with graphite monochromated Mo- $\text{K}\alpha$ radiation.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 25 carefully centered reflections in the range $39.02 < 2\theta < 39.94^\circ$ corresponded to a primitive orthorhombic cell with dimensions:

$$\begin{aligned}a &= 15.798(2) \text{ \AA} \\b &= 20.248(3) \text{ \AA} \\c &= 10.101(2) \text{ \AA} \\V &= 3231.2(9) \text{ \AA}^3\end{aligned}$$

For $Z = 4$ and F.W. = 594.89, the calculated density is 1.223 g/cm^3 . The systematic absences of:

$$\begin{aligned}h00: & h \pm 2n \\0k0: & k \pm 2n \\00l: & l \pm 2n\end{aligned}$$

uniquely determine the space group to be:

$$P2_12_12_1 \text{ (#19)}$$

The data were collected at a temperature of $20 \pm 1^\circ\text{C}$ using the ω - 2θ scan technique to a maximum 2θ value of 55.0° . Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.33° with a take-off angle of 6.0° . Scans of $(1.78 + 0.30 \tan \theta)^\circ$ were made at a speed of $0.0^\circ/\text{min}$ (in ω). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 5 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm and the crystal to detector distance was 235 mm. The computer-controlled slits were set to 9.0 mm (horizontal) and 13.0 mm (vertical).

Data Reduction

Of the 9650 reflections that were collected, 7423 were unique ($R_{\text{int}} = 0.025$). Over the course of data collection, the standards decreased by 0.4%. A linear correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ , for Mo-K α radiation is 1.805 cm^{-1} . An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.827 to 0.914. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction¹ was applied (coefficient = 0.006000).

Structure Solution and Refinement

The structure was solved by direct methods² and expanded using Fourier techniques³. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement⁴ on F^2 was based on 9638 observed reflections and 410 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \sum ||F_o| - |F_c|| / \sum |F_o| = 0.0394$$
$$wR2 = [\sum (w (F_o^2 - F_c^2)^2) / \sum w(F_o^2)^2]^{1/2} = 0.1533$$

The standard deviation of an observation of unit weight⁵ was 1.02. A Sheldrick weighting scheme was used. Plots of $S w (|F_o| - |F_c|)^2$ versus $|F_o|$, reflection order in data collection, $\sin \theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.45 and $-1.72 \text{ e}^-/\text{\AA}^3$, respectively. The absolute structure was deduced based on Flack parameter, 0.01(13), refined using 3272 Friedel pairs.⁶

Neutral atom scattering factors were taken from Cromer and Waber⁷. Anomalous dispersion effects were included in F_{calc} ⁸; the values for Df' and Df'' were those of Creagh and McAuley⁹. The values for the mass attenuation coefficients are those of Creagh and Hubbell¹⁰. All calculations were performed using the CrystalStructure^{11,12} crystallographic software package.

References

- (1) Larson, A. C. (1970), *Crystallographic Computing*, 291-294. F. R. Ahmed, ed. Munksgaard, Copenhagen (equation 22, with V replaced by the cell volume).
- (2) SHELX97: Sheldrick, G. M. (1997).
- (3) DIRDIF99: Beurskens, P. T., Admiraal, G., Beurskens, G., Bosman, W. P., de Gelder, R., Israel, R. and Smits, J. M. M. (1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
- (4) Least Squares function minimized:
$$\sum w(F_o^2 - F_c^2)^2 \quad \text{where } w = \text{Least Squares weights.}$$
- (5) Standard deviation of an observation of unit weight:
$$[\sum w(F_o^2 - F_c^2)^2 / (N_o - N_v)]^{1/2}$$

where: N_o = number of observations
 N_v = number of variables
- (6) Flack, H. D. (1983), *Acta Cryst.* A39, 876-881.

- (7) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).
- (8) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).
- (9) Creagh, D. C. & McAuley, W. J. ; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).
- (10) Creagh, D. C. & Hubbell, J. H.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).
- (11) CrystalStructure 3.8: Crystal Structure Analysis Package, Rigaku and Rigaku/MSO (2000-2006). 9009 New Trails Dr. The Woodlands TX 77381 USA.
- (12) CRYSTALS Issue 11: Carruthers, J.R., Rollett, J.S., Betteridge, P. W., Kinna, D., Pearce, L., Larsen, A., and Gabe, E. Chemical Crystallography Laboratory, Oxford, UK. (1999)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C ₃₆ H ₃₀ Si ₃ O ₃
Formula Weight	594.89
Crystal Color, Habit	colorless, prismatic
Crystal Dimensions	0.60 X 0.60 X 0.50 mm
Crystal System	orthorhombic
Lattice Type	Primitive
No. of Reflections Used for Unit	
Cell Determination (2 θ range)	25 (39.0 - 39.9 $^{\circ}$)
Omega Scan Peak Width	
at Half-height	0.33 $^{\circ}$
Lattice Parameters	$a = 15.798(2) \text{ \AA}$ $b = 20.248(3) \text{ \AA}$ $c = 10.101(2) \text{ \AA}$ $V = 3231.2(9) \text{ \AA}^3$
Space Group	$P2_12_12_1$ (#19)
Z value	4
D _{calc}	1.223 g/cm ³
F ₀₀₀	1248.00
$\mu(\text{MoK}\alpha)$	1.805 cm ⁻¹

B. Intensity Measurements

Diffractometer	Rigaku AFC7S
Radiation	MoK α ($\lambda = 0.71069 \text{ \AA}$) graphite monochromated
Attenuator	Zr foil (factor = 9.04)
Take-off Angle	6.0 $^\circ$
Detector Aperture	13.0 mm horizontal 9.0 mm vertical
Crystal to Detector Distance	235 mm
Temperature	20.0 $^\circ$ C
Scan Type	ω -2 θ
Scan Rate	0.0 $^\circ$ /min (in ω) (up to 5 scans)
Scan Width	(1.78 + 0.30 tan θ) $^\circ$
2 θ_{max}	55.0 $^\circ$
No. of Reflections Measured	Total: 9650 Unique: 7413 ($R_{\text{int}} = 0.025$) Friedel pairs: 3272
Corrections	Lorentz-polarization Absorption (trans. factors: 0.827 - 0.914) Decay (0.43% decline) Secondary Extinction (coefficient: 6.00000e-003)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELX97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma w (F_o^2 - F_c^2)^2$
Least Squares Weight	1/[0.0010 F_o^2 +3.0000s(F_o^2)+0.5000]/(4 F_o^2)
2 θ_{max} cutoff	55.0 $^\circ$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	9638
No. Variables	410
Reflection/Parameter Ratio	23.51
Residuals: R_1 ($I > 2.00s(I)$)	0.0394
Residuals: R (All reflections)	0.0603
Residuals: wR_2 (All reflections)	0.1533

Goodness of Fit Indicator	1.023
Flack Parameter	0.01(13)
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	1.45 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-1.72 e ⁻ /Å ³

Crystallographic analysis of hexaphenylcyclotrisiloxane *M*-4

Data Collection

A colorless prismatic crystal of C₃₆H₃₀Si₃O₃ having approximate dimensions of 0.70 x 0.65 x 0.60 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC7S diffractometer with graphite monochromated Mo-K α radiation.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 25 carefully centered reflections in the range $38.97 < 2\theta < 39.92^\circ$ corresponded to a primitive orthorhombic cell with dimensions:

$$\begin{aligned}a &= 15.801(2) \text{ \AA} \\b &= 20.2479(17) \text{ \AA} \\c &= 10.1003(15) \text{ \AA} \\V &= 3231.4(7) \text{ \AA}^3\end{aligned}$$

For $Z = 4$ and F.W. = 594.89, the calculated density is 1.223 g/cm³. The systematic absences of:

$$\begin{aligned}h00: & h \pm 2n \\0k0: & k \pm 2n \\00l: & l \pm 2n\end{aligned}$$

uniquely determine the space group to be:

$$P2_12_12_1 \text{ (#19)}$$

The data were collected at a temperature of $20 \pm 1^\circ\text{C}$ using the ω - 2θ scan technique to a maximum 2θ value of 55.0° . Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.34° with a take-off angle of 6.0° . Scans of $(1.68 + 0.30 \tan \theta)^\circ$ were made at a speed of $0.0^\circ/\text{min}$ (in ω). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 5 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm and the crystal to detector distance was 235 mm. The computer-controlled slits were set to 9.0 mm (horizontal) and 13.0 mm (vertical).

Data Reduction

Of the 8298 reflections that were collected, 7419 were unique ($R_{\text{int}} = 0.010$). Over the course of data collection, the standards decreased by 0.2%. A linear correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ , for Mo-K α radiation is 1.805 cm⁻¹. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.784 to 0.897. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods¹ and expanded using Fourier techniques². The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement³ on F^2 was based on 8288 observed reflections and 410 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \sum ||F_{\text{ol}} - |F_{\text{cl}}|| / \sum |F_{\text{ol}}| = 0.0386$$

$$wR2 = [\sum (w (F_{\text{o}}^2 - F_{\text{c}}^2)^2) / \sum w(F_{\text{o}}^2)^2]^{1/2} = 0.1398$$

The standard deviation of an observation of unit weight⁴ was 0.98. A Sheldrick weighting scheme was used. Plots of $\sum w (|F_{\text{ol}} - |F_{\text{cl}}||)^2$ versus $|F_{\text{ol}}|$, reflection order in data collection, $\sin \theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.54 and -0.56 e⁻/Å³, respectively. The absolute structure was deduced based on Flack parameter, 0.02(10), refined using 3270 Friedel pairs.⁵

Neutral atom scattering factors were taken from Cromer and Waber⁶. Anomalous dispersion effects were included in F_{calc} ⁷; the values for D_{f} and D_{f}'' were those of Creagh and McAuley⁸. The values for the mass attenuation coefficients are those of Creagh and Hubbell⁹. All calculations were performed using the CrystalStructure^{10,11} crystallographic software package.

References

- (1) SHELX97: Sheldrick, G. M. (1997).
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- (5) Flack, H. D. (1983), Acta Cryst. A39, 876-881.
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Lattice Type	Primitive
No. of Reflections Used for Unit	
Cell Determination (2θ range)	25 (39.0 - 39.9 $^\circ$)
Omega Scan Peak Width at Half-height	0.34 $^\circ$
Lattice Parameters	$a = 15.801(2) \text{ \AA}$ $b = 20.2479(17) \text{ \AA}$ $c = 10.1003(15) \text{ \AA}$ $V = 3231.4(7) \text{ \AA}^3$
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Z value	4
D_{calc}	1.223 g/cm 3
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Detector Aperture	13.0 mm horizontal 9.0 mm vertical
Crystal to Detector Distance	235 mm
Temperature	20.0 °C
Scan Type	ω - 2θ
Scan Width	(1.68 + 0.30 tan θ)°
$2\theta_{\max}$	55.0°
No. of Reflections Measured	Total: 8298 Unique: 7409 ($R_{\text{int}} = 0.010$) Friedel pairs: 3270
Corrections	Lorentz-polarization Absorption (trans. factors: 0.784 - 0.897) Decay (0.17% decline)

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Least Squares Weights	1/[0.0027 F_o^2 +1.0000 $\sigma(F_o^2)$]/(4 F_o^2)
$2\theta_{\max}$ cutoff	55.0°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	8288
No. Variables	410
Reflection/Parameter Ratio	20.21
Residuals: R_1 ($I > 2.00\sigma(I)$)	0.0386
Residuals: R (All reflections)	0.0511
Residuals: wR_2 (All reflections)	0.1398
Goodness of Fit Indicator	0.984
Flack Parameter	0.02(10)
Max Shift/Error in Final Cycle	0.000

Maximum peak in Final Diff. Map	$0.54 \text{ e}^-/\text{\AA}^3$
Minimum peak in Final Diff. Map	$-0.56 \text{ e}^-/\text{\AA}^3$