

Silylene-mediated Polarity Reversal of Dienoates: Addition of Dienoates to Aldehydes at the δ -Position to form *trans*-Dioxasilacyclononenes

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Supporting Information

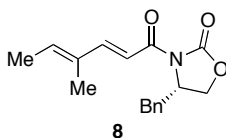
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I. General Experimental Considerations

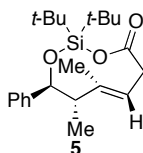
Melting points were obtained using a Büchi 510 melting point apparatus and were reported uncorrected. Gas chromatography-mass spectrometry (GCMS) was performed on a Thermo-Finnigan Trace Mass Spectrometer Plus quadrupole system with a fused silica capillary column (30 m x 0.32 mm x 0.25 mm) wall-coated with DB-5 (J & W Scientific) using electron ionization (70 eV). Analytical thin layer chromatography was performed on EM reagents 0.25 mm silica gel 60-F plates. Liquid chromatography was performed using forced flow (flash chromatography) of the indicated solvent system on EM reagents silica gel (SiO₂) 60 (230–400) mesh. ¹H NMR and ¹³C NMR spectra were recorded at 25 °C at 400 and 100, 500 and 125, and 600 and 150 MHz, respectively, using Bruker DRX 400, DRX 500, or Bruker Avance 600 spectrometers, as indicated. The ¹H NMR data are reported as follows: chemical shift in ppm from internal tetramethylsilane on the δ scale, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, qn = quintet, sext = sextet, sept = septet, m = multiplet, and br = broad), coupling constants (Hz), and integration. The ¹³C NMR chemical shifts are reported in ppm from tetramethylsilane on the δ scale, using tetramethylsilane as an internal standard. High resolution mass spectra were acquired on a LCT Premier Quadrupole Time of Flight Spectrometer, and were obtained by peak matching. Microanalyses were performed by Atlantic Microlabs, Norcross, GA. Cyclohexene silacyclopropane **2**¹ was stored and manipulated in an Innovative Technologies nitrogen atmosphere dry box. All reaction mixtures to form vinyl oxasilacyclopentenes, unless otherwise specified, were prepared in the dry box. All other reactions unless specified were performed under an atmosphere of nitrogen or argon in glassware that had been flame-dried under a stream of nitrogen or under vacuum. Solvents were distilled or filtered before use. Unless otherwise noted, all reagents and substrates were commercially available. Dienoates that were not commercially available were prepared following literature procedures.^{2,3}

II. Substrate Preparation



(S)-4-Benzyl-3-((2E,4E)-4-methylhexa-2,4-dienoyl)oxazolidin-2-one (8). To a solution (2E,4E)-4-methylhexa-2,4-dienoic acid⁴ (0.631 g, 5.00 mmol) in benzene (20.0 mL) was added oxalyl chloride (0.86 mL, 10 mmol). The mixture was allowed to stir for 20 h. The mixture was concentrated *in vacuo* to afford (2E,4E)-4-methylhexa-2,4-dienoyl chloride, which was carried onto the next step without purification. To a cooled (−78 °C) solution of (S)-4-benzylloxazolidin-2-one (0.886 g, 5.00 mmol) in THF (25.0 mL) was added *n*-BuLi (2.00 mL, 2.50 M, 5.00 mmol). The mixture was allowed to stir at −78 °C for 10 min. A solution of the unpurified (2E,4E)-4-methylhexa-2,4-dienoyl chloride in THF (8.0 mL) was added. The mixture was allowed to warm slowly to rt over 16 h. The reaction mixture was diluted with a saturated aqueous NH₄Cl (50.0 mL) and extracted with CH₂Cl₂ (3 x 20 mL). The organic layers were combined, washed with brine, filtered, and concentrated *in vacuo* to a yellow oil. The oil was purified by flash chromatography (40:60 EtOAc:hexanes) to afford the product as a colorless solid (0.738 g, 52%): mp 99–101 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.57 (d, *J* = 15.3 Hz, 1H), 7.37 – 7.22 (m, 6H), 6.15 – 6.09 (m, 1H), 4.80 – 4.74 (m, 1H), 4.22 (t, *J* = 8.3 Hz, 1H), 4.18 (dd, *J* = 9.0, 3.1 Hz, 1H), 3.36 (dd, *J* = 13.5, 3.3 Hz, 1H), 2.82 (dd, *J* = 13.4, 9.5 Hz, 1H), 1.87 – 1.86 (m, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 218.4, 166.0, 151.8, 138.6, 135.7, 134.9, 129.7, 129.2, 127.5, 114.5, 66.3, 55.7, 38.3, 15.1, 12.3; IR (thin film) 3030, 2920, 1778, 1676, 1603, 1352 cm^{−1}; HRMS (ESI) *m/z* calcd for C₁₇H₁₉NNaO₃ (M + Na)⁺ 308.1263, found 308.1269. Anal. Calcd for C₁₇H₁₉NO₃: C, 71.56; H, 6.71. Found: C, 71.54; H, 6.86.

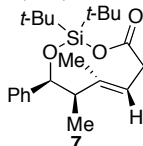
III. Formation of *trans*-Dioxasilacyclononenes



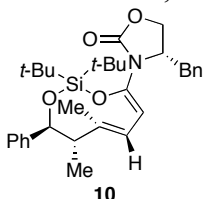
Representative procedure for the synthesis of *trans*-dioxasilacyclononenes under thermal conditions (cyclononene 5). To an NMR tube was added AgO₂CCF₃ (0.0002 g, 0.001 mmol). A solution of ethyl (2E,4E)-4-methylhexa-2,4-dienoate (0.015 g, 0.10 mmol) in toluene-*d*₈ (0.25 mL) was added followed by a solution of cyclohexene silacyclopropane **2** (0.028 g, 0.12 mmol) and PhSiMe₃ (internal standard, 0.008 g, 0.05 mmol) in toluene-*d*₈ (0.25 mL). The mixture was allowed to sit at room temperature for 30 min. Benzaldehyde (0.031 mL, 0.30 mmol) was added, and the mixture was heated to 100 °C for 18 h. The mixture was cooled to rt, filtered through a plug of SiO₂, and concentrated *in vacuo* to afford an oil. ¹H NMR spectroscopy and GCMS of the unpurified reaction mixture revealed formation of the product as a single diastereomer. The oil was purified by flash chromatography (10:90 EtOAc:hexanes) to afford cyclononene **5** a colorless solid (0.029 g, 77%).

Representative procedure for the synthesis of *trans*-dioxasilacyclononenes under Lewis acid conditions (cyclononene 5). This reaction can be scaled up (see the synthesis of **21**, p. S-6). To an NMR tube was added AgO₂CCF₃ (0.0002 g, 0.001 mmol). A solution of ethyl (2E,4E)-4-methylhexa-2,4-dienoate (0.015 g, 0.10 mmol) in toluene-*d*₈ (0.25 mL) was added followed by a solution of cyclohexene silacyclopropane **2** (0.028 g, 0.12 mmol) and PhSiMe₃ (internal standard, 0.008 g, 0.05 mmol) in toluene-*d*₈ (0.25 mL). The mixture was allowed to sit at room temperature for 30 min. Benzaldehyde (0.031 mL, 0.30 mmol) was added followed by SnBr₄ (0.004 g, 0.01 mmol). After the mixture was allowed to sit for 3 h, it was filtered through a plug of SiO₂ and concentrated *in vacuo* to afford an oil. ¹H NMR spectroscopy and GCMS of the unpurified reaction mixture revealed formation

of the product as a single diastereomer. The oil was purified by flash chromatography (10:90 EtOAc:hexanes) to afford cyclononene **5** a colorless solid (0.014 g, 37%): mp 103-105 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.42 – 7.35 (m, 5H), 5.60 (dd, *J* = 10.8, 5.6 Hz, 1H), 4.65 (d, *J* = 9.6 Hz, 1H), 3.55 (dd, *J* = 17.1, 10.8 Hz, 1H), 3.20 (dd, *J* = 17.1, 5.8 Hz, 1H), 2.53 – 2.47 (m, 1H), 1.74 (s, 3H), 1.08 (s, 9H), 1.04 (s, 9H), 0.77 (d, *J* = 7.0 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 169.5, 142.3, 140.7, 128.2, 127.6, 126.7, 121.1, 79.5, 51.9, 36.0, 28.0, 27.4, 21.0, 20.9, 13.7, 11.6; IR (thin film) 3064, 3032, 2937, 1728, 1471, 1203 cm⁻¹; HRMS (ESI) *m/z* calcd for C₂₂H₃₄NaO₃Si (M + Na)⁺ 397.2175, found 397.2177. Anal. Calcd for C₂₂H₃₄O₃Si: C, 70.54; H, 9.15. Found: C, 70.77; H, 9.12.

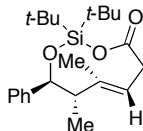


Cyclononene 7. The representative procedure for the formation of *trans*-dioxasilacyclononene was followed using ethyl (2*E*,4*Z*)-4-methylhexa-2,4-dienoate (0.015 g, 0.10 mmol). The reaction under thermal conditions afforded cyclononene **7** as a colorless oil (0.025 g, 67%): ¹H NMR (400 MHz, CDCl₃) δ 7.38 – 7.25 (m, 5H), 5.49 (dd, *J* = 11.1, 5.6 Hz, 1H), 5.24 (d, *J* = 2.0 Hz, 1H), 3.48 (dd, *J* = 16.9, 11.1 Hz, 1H), 3.18 (dd, *J* = 16.8, 5.6 Hz, 1H), 2.49-2.43 (m, 1H), 1.91 (s, 3H), 1.17 (s, 9H), 0.96 (s, 9H), 0.80 (d, *J* = 6.9 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.4, 142.7, 142.2, 128.3, 127.0, 125.5, 117.4, 75.4, 49.7, 36.2, 28.3, 28.0, 21.7, 21.3, 18.1, 9.9; IR (thin film) 3062, 2970, 1730, 1473, 1369, 654 cm⁻¹; HRMS (ESI) *m/z* calcd for C₂₂H₃₄NaO₃Si (M + Na)⁺ 397.2175, found 397.2181. Anal. Calcd for C₂₂H₃₄O₃Si: C, 70.54; H, 9.15. Found: C, 70.53; H, 9.31.



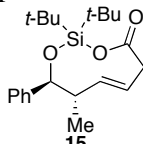
Cyclononene 10. The representative procedure for the formation of *trans*-dioxasilacyclononene was followed using (*S*)-4-benzyl-3-((2*E*,4*E*)-4-methylhexa-2,4-dienyl)oxazolidin-2-one (0.029 g, 0.10 mmol) and AgO₂CCF₃ (0.001 g, 0.005 mmol). The reaction thermal conditions afforded cyclononene **10** as a colorless solid (0.039 g, 73%). Cyclononene **10** appears as 1:1 mixture of isomers by ¹H and ¹³C NMR spectroscopic analysis at room temperature. GCMS analysis of cyclononene **10** shows a mixture diastereomers (96:4 dr) that is consistent with the diastereoselectivity found with silylene transfer to (*S,E*)-4-benzyl-3-but-2-enoyloxazolidin-2-one. Relative configuration of cyclononene **10** was determined by X-ray crystallography. We hypothesized that cyclononene **10** exists in two equal energy conformation at room temperature. ¹H NMR spectroscopy of cyclononene **10** at elevated temperatures shows the initially 1:1 mixture of isomers coalesce to one isomer: ¹H NMR (400 MHz, tol-*d*₈, 100 °C) δ 7.26 – 6.95 (m, 10H), 5.83 (s, 1H), 5.62 (br s, 1H), 4.60 – 4.50 (m, 1H), 4.19 (br s, 1H), 3.72 – 3.60 (m, 2H), 3.13 (dd, *J* = 13.9, 3.8 Hz, 1H), 2.54 (dd, *J* = 13.8, 9.5 Hz, 1H), 2.21 – 2.17 (m, 1H), 1.88 (s, 3H), 1.11 (s, 9H), 1.04 (s, 9H), 0.96 – 0.94 (m, 3H). Cooling the sample back down to room temperature reverts it back to a 1:1 mixture: mp 154-155 °C; ¹H NMR (400 MHz, C₆D₆) δ 7.28 – 6.90 (m, 20H), 6.03 (s, 1H), 5.94 (s, 1H), 5.83 (s, 1H), 5.66 (s, 1H), 4.69 (d, *J* = 9.7 Hz, 1H), 4.47 (d, *J* = 9.6 Hz, 1H), 4.35 – 4.31 (m, 1H), 3.99 – 3.94 (m, 1H), 3.55 – 3.45 (m, 4H), 3.11 (dd, *J* = 13.5, 3.6 Hz, 1H), 3.04 (dd, *J* = 13.6, 3.6 Hz, 1H), 2.52 – 2.37 (m, 3H), 2.25 – 2.17 (m, 1H), 2.02 (s, 3H), 1.89 (s, 3H), 1.19 (s, 9H), 1.15 (s, 9H), 1.11 (s, 9H), 1.06 (s, 9H), 0.88 (d, *J* = 6.9 Hz, 3H), 0.68 (d, *J* = 7.0 Hz, 3H); ¹³C NMR (100 MHz, C₆D₆) δ 155.1, 154.8, 149.1, 143.3, 142.9, 142.1, 141.0, 140.3, 136.1, 136.0, 129.52, 129.47, 129.10, 129.05, 128.52, 128.50, 128.2, 127.9, 127.33, 127.30, 127.2, 126.9, 123.0, 122.6, 115.7, 101.9,

101.7, 88.2, 79.9, 66.0, 65.8, 57.3, 55.9, 52.4, 49.5, 39.0, 38.6, 28.84, 28.81, 28.6, 28.3, 24.8, 22.7, 21.8, 21.2, 14.8, 13.52, 13.50; IR (thin film) 2926, 2856, 1768, 1643, 1456, 1092 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{32}\text{H}_{43}\text{NNaO}_4\text{Si}$ ($M + \text{Na}$)⁺ 556.2859, found 556.2860. Anal. Calcd for $\text{C}_{32}\text{H}_{43}\text{NO}_4\text{Si}$: C, 72.00; H, 8.12. Found: C, 72.20; H, 8.19.



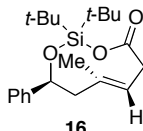
(-)-5

Cyclononene (-)-5. To a solution of cyclononene **10** (0.037 g, 0.070 mmol) in ether (0.7 mL) was added a solution of HCl (1.0 mL, 1.0 M, 1.0 mmol). The mixture was stirred for 1 h. The mixture was diluted with ether (2.0 mL). The layers were separated, and the organic layer was washed with a saturated aqueous solution of NaHCO_3 , washed with brine, dried over MgSO_4 , filtered, and concentrated *in vacuo* to afford a colorless solid (0.026g, 100%): $[\alpha]_{\text{D}}^{25} - 36.6^\circ$ (c 1.00, CH_2Cl_2); ^1H and ^{13}C NMR spectroscopic data matched those reported above.



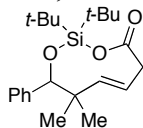
15

Cyclononene 15. The representative procedure for the formation of *trans*-dioxasilacyclononene was followed using ethyl sorbate (0.014 g, 0.10 mmol). The reaction mixture was heated to 100 °C for 5 d to afford cyclononene **15** as a colorless solid (0.021 g, 59%): mp 100-102 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.37 – 7.28 (m, 5H), 5.69 (ddd, $J = 15.2, 9.4, 5.9$ Hz, 1H), 5.47 (dd, $J = 15.2, 9.8$ Hz, 1H), 4.52 (d, $J = 9.5$ Hz, 1H), 3.22 – 3.19 (m, 2H), 2.36 (tq, $J = 9.7, 6.6$ Hz, 1H), 1.01 (s, 18H), 0.80 (d, $J = 6.7$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 169.3, 142.0, 140.3, 128.2, 127.7, 126.8, 125.4, 81.4, 47.4, 40.7, 28.0, 27.2, 20.74, 20.68, 15.9; IR (thin film) 3034, 2935, 1730, 1471, 1093, 972 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{21}\text{H}_{32}\text{NaO}_3\text{Si}$ ($M + \text{Na}$)⁺ 383.2018, found 383.2025. Anal. Calcd for $\text{C}_{21}\text{H}_{32}\text{O}_3\text{Si}$: C, 69.95; H, 8.95. Found: C, 70.05; H, 9.01.



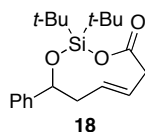
16

Cyclononene 16. The representative procedure for the formation of *trans*-dioxasilacyclononene was followed using ethyl (*E*)-4-methylpenta-2,4-dienoate (0.014 g, 0.10 mmol). The reaction mixture was heated to 100 °C for 2 d to afford cyclononene **16** as a colorless solid (0.019 g, 53%): mp 83-85 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.43 – 7.32 (m, 5H), 5.54 (ddd, $J = 11.2, 5.5, 0.6$ Hz, 1H), 5.13 (dd, $J = 9.6, 3.6$ Hz, 1H), 3.49 (dd, $J = 17.0, 11.2$ Hz, 1H), 3.19 (dd, $J = 17.0, 5.5$ Hz, 1H), 2.41 – 2.34 (m, 2H), 1.88 (s, 3H), 1.16 (s, 9H), 1.05 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ 169.2, 144.1, 137.0, 128.4, 127.3, 125.1, 121.6, 74.2, 51.8, 36.2, 28.1, 27.5, 21.1, 21.0, 16.2; IR (thin film) 3030, 2937, 1730, 1473, 1201, 1086 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{21}\text{H}_{32}\text{NaO}_3\text{Si}$ ($M + \text{Na}$)⁺ 383.2018, found 383.2020. Anal. Calcd for $\text{C}_{21}\text{H}_{32}\text{O}_3\text{Si}$: C, 69.95; H, 8.95. Found: C, 69.78; H, 9.08.

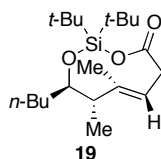


17

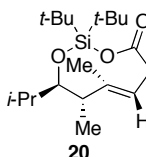
Cyclononene 17. The representative procedure for the formation of *trans*-dioxasilacyclononene was followed using ethyl (*E*)-5-methylhexa-2,4-dienoate (0.015 g, 0.10 mmol). The reaction mixture was heated to 100 °C for 10 d to afford cyclononene **17** as a colorless solid (0.014 g, 38%): mp 104-106 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.35 – 7.27 (m, 5H), 5.67 (d, *J* = 15.6 Hz, 1H), 5.58 (ddd, *J* = 15.4, 9.4, 5.5 Hz, 1H), 4.76 (s, 1H), 3.27 – 3.20 (m, 2H), 1.09 (s, 9H), 0.95 (s, 9H), 0.93 (s, 3H), 0.93 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 169.5, 146.0, 139.5, 127.7, 127.5, 127.4, 121.1, 82.1, 42.9, 41.0, 28.0, 27.4, 25.3, 21.0, 20.9, 16.5; IR (thin film) 3030, 2935, 2862, 1732, 1473, 1095 cm⁻¹; HRMS (ESI) *m/z* calcd for C₂₂H₃₄NaO₃Si (M + Na)⁺ 397.2175, found 397.2179. Anal. Calcd for C₂₂H₃₄O₃Si: C, 70.54 H, 9.15. Found: C, 70.70; H, 9.21.



Cyclononene 18. The representative procedure for the formation of *trans*-dioxasilacyclononene was followed using ethyl (*E*)-penta-2,4-dienoate (0.013 g, 0.10 mmol). The reaction mixture was heated to 100 °C for 5 d to afford cyclononene **18** as a colorless oil (0.013 g, 37%): ¹H NMR (500 MHz, CDCl₃) δ 7.37 – 7.27 (m, 5H), 5.75 (ddd, *J* = 15.1, 10.7, 4.3 Hz, 1H), 5.66 (dt, *J* = 15.2, 7.5 Hz, 1H), 5.04 (dd, *J* = 10.9, 2.4 Hz, 1H), 3.29 (s, 1H), 3.27 (s, 1H), 2.54 – 2.50 (m, 1H), 2.22 (dt, *J* = 12.6, 10.7 Hz, 1H), 1.09 (s, 9H), 1.02 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ 169.2, 143.9, 133.9, 128.5, 127.9, 127.4, 125.2, 75.6, 44.7, 40.9, 28.1, 27.5, 21.0, 20.9; IR (thin film) 3032, 2947, 1730, 1471, 1230, 827 cm⁻¹; HRMS (ESI) *m/z* calcd for C₂₀H₃₀NaO₃Si (M + Na)⁺ 369.1862, found 369.1859. Anal. Calcd for C₂₀H₃₀O₃Si: C, 69.32; H, 8.73. Found: C, 69.06; H, 8.75.

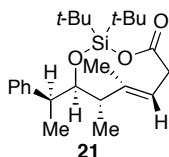


Cyclononene 19. The representative procedure for the formation of *trans*-dioxasilacyclononene was followed using valeraldehyde (0.026 g, 0.30 mmol). Under thermal conditions, the reaction mixture was heated to 100 °C for 18 h to afford cyclononene **19** as a colorless oil (0.026 g, 72%). Under Lewis acid catalysis, the reaction mixture was allowed to sit at rt for 3 h, and cyclononene **19** was isolated as a colorless oil (0.013 g, 37%): ¹H NMR (500 MHz, CDCl₃) δ 5.33 (dd, *J* = 10.7, 5.9 Hz, 1H), 3.89 (ddd, *J* = 9.7, 4.6, 3.5 Hz, 1H), 3.40 (dd, *J* = 17.0, 10.7 Hz, 1H), 3.04 (dd, *J* = 17.1, 5.9 Hz, 1H), 2.31 (dq, *J* = 9.7, 7.0 Hz, 1H), 1.73-1.66 (m, 2H), 1.57 (s, 3H), 1.55-1.33 (m, 4H), 1.05 (s, 9H), 1.02 (s, 9H), 0.98 (d, *J* = 6.9 Hz, 3H), 0.93 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 169.7, 141.5, 120.0, 76.3, 47.8, 35.8, 34.1, 28.2, 27.5, 25.6, 23.2, 21.4, 21.2, 14.1, 13.8, 11.5; IR (thin film) 2935, 2862, 1730, 1471, 1082, 976 cm⁻¹; HRMS (ESI) *m/z* calcd for C₂₀H₃₈NaO₃Si (M + Na)⁺ 377.2488, found 377.2480. Anal. Calcd for C₂₀H₃₈O₃Si: C, 67.74; H, 10.80. Found: C, 67.94; H, 11.01.

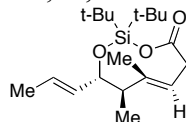


Cyclononene 20. The representative procedure for the formation of *trans*-dioxasilacyclononene was followed using isobutyraldehyde (0.022 g, 0.30 mmol). Under thermal conditions, the reaction mixture was heated to 130 °C for 3 d in a flame sealed NMR tube to afford cyclononene **20** as a colorless solid (0.025 g, 73%). Under Lewis acid catalysis, the reaction mixture was allowed to sit at rt for 18 h to afford cyclononene **20** as a colorless solid (0.014 g, 40%): mp 68-71 °C; ¹H NMR (500 MHz, CDCl₃) δ

5.35 (ddd, $J = 10.6, 5.9, 1.4$ Hz, 1H), 3.87 (dd, $J = 9.9, 1.8$ Hz, 1H), 3.38 (dd, $J = 17.0, 10.6$ Hz, 1H), 3.02 (dd, $J = 17.0, 5.9$ Hz, 1H), 2.39 (dq, $J = 9.8, 6.9$ Hz, 1H), 1.92 (dtd, $J = 13.8, 6.9, 1.8$ Hz, 1H), 1.59 (d, $J = 1.4$ Hz, 3H), 1.11 (d, $J = 7.0$ Hz, 3H), 1.08 (s, 9H), 1.05 (s, 9H), 0.97 (d, $J = 6.9$ Hz, 3H), 0.92 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.7, 142.2, 120.3, 81.4, 47.2, 35.9, 30.4, 28.6, 27.9, 22.3, 22.1, 21.9, 14.4, 14.2, 11.8; IR (thin film) 2970, 2862, 1730, 1471, 1205, 1068 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{36}\text{NaO}_3\text{Si}$ ($\text{M} + \text{Na}$) $^+$ 363.2332, found 363.2328. Anal. Calcd for $\text{C}_{19}\text{H}_{36}\text{O}_3\text{Si}$: C, 67.01; H, 10.65. Found: C, 67.27; H, 10.62.

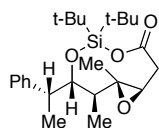


Cyclononene 21. The representative procedure for the formation of *trans*-dioxasilacyclononene under thermal conditions was followed using (\pm)-2-phenylpropanal (0.040 g, 0.30 mmol). Under thermal conditions, the reaction mixture was heated to 130 $^\circ\text{C}$ for 5 d in a flame sealed NMR tube to afford cyclononene **21** as a colorless solid (0.029 g, 72%). Under Lewis acid catalysis: to AgO_2CCF_3 (0.004 g, 0.02 mmol) was added a solution of ethyl (*2E,4E*)-4-methylhexa-2,4-dienoate (0.308 g, 2.00 mmol) in toluene (10.0 mL), and cyclohexene silacyclopropane **2** (0.561 g, 2.5 mmol) was added dropwise. The mixture was allowed to stir at room temperature for 30 min. (\pm)-2-Phenylpropanal (0.805 g, 6.00 mmol) was added followed by SnBr_4 (0.088 g, 0.20 mmol). After the mixture was allowed to stir for 18 h, 60 mL of a saturated aqueous solution of NaHCO_3 was added. The layers were separated, and the aqueous layer was extracted with CH_2Cl_2 (3 x 25 mL). The organic layers were combined, washed with brine, filtered, and concentrated *in vacuo* to afford an oil. ^1H NMR spectroscopy and GCMS of the unpurified reaction mixture revealed formation of a single diastereomer. The oil was purified by flash chromatography (10:90 EtOAc:hexanes) to afford the product a colorless solid (0.754 g, 94%). The relative configuration of cyclononene **21** was determined by X-ray crystallography: mp 101-104 $^\circ\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.44 – 7.16 (m, 5H), 5.41 (ddd, $J = 10.2, 6.3, 1.2$ Hz, 1H), 4.20 (dd, $J = 9.8, 1.7$ Hz, 1H), 3.38 (dd, $J = 17.2, 10.4$ Hz, 1H), 3.13 (qd, $J = 7.1, 1.5$ Hz, 1H), 3.02 (dd, $J = 17.2, 6.1$ Hz, 1H), 2.54 (dq, $J = 9.8, 6.9$ Hz, 1H), 1.61 (d, $J = 1.3$ Hz, 3H), 1.37 (d, $J = 7.1$ Hz, 3H), 1.15 (d, $J = 6.9$ Hz, 3H), 1.02 (s, 9H), 0.49 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.5, 144.9, 142.0, 128.6, 128.5, 126.5, 120.6, 82.4, 47.7, 40.6, 35.8, 28.0, 27.6, 21.8, 21.6, 14.9, 11.8, 10.5; IR (thin film) 2937, 2860, 1728, 1471, 1207, 1092 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{24}\text{H}_{38}\text{NaO}_3\text{Si}$ ($\text{M} + \text{Na}$) $^+$ 425.2488, found 425.2485. Anal. Calcd for $\text{C}_{24}\text{H}_{38}\text{O}_3\text{Si}$: C, 71.59; H, 9.51. Found: C, 71.36; H, 9.51.

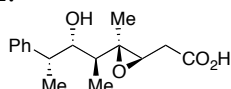


Cyclononene 22. The representative procedure for the formation of *trans*-dioxasilacyclononene was followed using crotonaldehyde (0.021 g, 0.30 mmol). Under thermal conditions, the reaction mixture was heated to 100 $^\circ\text{C}$ for 18 h to afford cyclononene **22** as a colorless oil (0.027 g, 80%): ^1H NMR (400 MHz, CDCl_3) δ 5.69 – 5.60 (m, 1H), 5.44 – 5.35 (m, 2H), 4.06 (dd, $J = 9.3, 7.3$ Hz, 1H), 3.42 (dd, $J = 17.1, 10.7$ Hz, 1H), 3.07 (dd, $J = 17.2, 6.0$ Hz, 1H), 2.22 – 2.16 (m, 1H), 1.73 (dd, $J = 6.5, 1.0$ Hz, 3H), 1.58 (s, 3H), 1.03 (s, 9H), 1.02 (s, 9H), 0.94 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.8, 141.0, 132.1, 127.2, 120.6, 78.1, 50.1, 36.0, 28.2, 27.7, 21.2, 21.1, 17.9, 13.9, 11.6; IR (thin film) 2937, 2862, 1732, 1473, 1201, 1090 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{34}\text{NaO}_3\text{Si}$ ($\text{M} + \text{Na}$) $^+$ 361.2175, found 361.2179. Anal. Calcd for $\text{C}_{19}\text{H}_{34}\text{O}_3\text{Si}$: C, 67.40; H, 10.12. Found: C, 67.82; H, 10.25.

IV. Functionalization of *trans*-Dioxasilacyclononenes



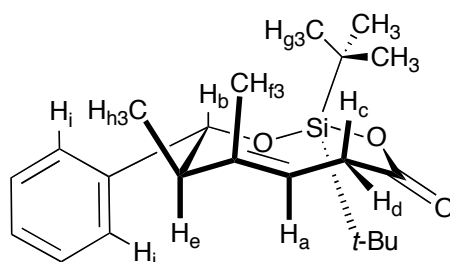
Epoxide 23'. To a solution of cyclononene **21** (0.040 g, 0.10 mmol) in CH_2Cl_2 (1.0 mL) was added *m*-CPBA (0.074 g, 70% wt, 0.30 mmol). The mixture stirred for 30 min, and then was concentrated *in vacuo*. The residue was purified by flash chromatography (10:90 EtOAc:hexanes) to afford the product as a colorless solid (0.029 g, 68%): mp 155-158 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.39 – 7.18 (m, 5H), 4.37 (dd, $J = 10.3, 1.7$ Hz, 1H), 3.14 – 3.09 (m, 3H), 2.47 (dd, $J = 17.7, 11.3$ Hz, 1H), 1.51 – 1.45 (m, 1H), 1.31 (d, $J = 7.2$ Hz, 3H), 1.31 (s, 3H), 1.19 (d, $J = 6.9$ Hz, 3H), 1.06 (s, 9H), 0.55 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 166.9, 144.2, 128.7, 128.6, 126.7, 82.2, 62.5, 61.8, 47.3, 40.8, 36.9, 28.0, 27.5, 21.59, 21.57, 13.6, 12.4, 10.2; IR (thin film) 2937, 2862, 1738, 1473, 1240, 1092 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{24}\text{H}_{38}\text{NaO}_4\text{Si}$ ($\text{M} + \text{Na}$) $^+$ 441.2437, found 441.2436. Anal. Calcd for $\text{C}_{24}\text{H}_{38}\text{O}_4\text{Si}$: C, 68.86; H, 9.15. Found: C, 68.99; H, 9.22.



Acid 23. To epoxide **23'** (0.057 g, 0.14 mmol) was added *n*-Bu₄NF (1.40 mL, 1.0 M in THF, 1.4 mmol). The mixture stirred for 3 d, and then it was diluted with 5 mL of H₂O followed by 1 mL of 1.0 N HCl solution. The mixture was extracted with MTBE (3 x 5 mL). The organic layers were combined, washed with brine, dried over MgSO₄, filtered, and concentrated *in vacuo* to afford an oil. The oil was purified by flash chromatography (10:90 MeOH: CH_2Cl_2) to afford the product as a colorless oil (0.023 g, 58%): ^1H NMR (400 MHz, CDCl_3) δ 7.33 – 7.20 (m, 5H), 4.19 (dd, $J = 9.1, 7.8$ Hz, 1H), 3.91 (dd, $J = 9.9, 2.9$ Hz, 1H), 3.01 – 2.97 (m, 1H), 2.76 (qn, $J = 7.2$ Hz, 1H), 2.39 (dd, $J = 15.5, 3.0$ Hz, 1H), 2.28 (dd, $J = 15.5, 10.0$ Hz, 1H), 1.31 (s, 3H), 1.30 (d, $J = 6.9$ Hz, 3H), 0.60 (d, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 176.2, 141.3, 128.7, 128.1, 127.2, 88.4, 85.7, 73.2, 46.2, 36.3, 35.3, 18.0, 16.9, 13.4; IR (thin film) 3417, 2967, 1714, 1454, 1282, 1072 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{22}\text{NaO}_4$ ($\text{M} + \text{Na}$) $^+$ 301.1416, found 301.1409.

V. Stereochemical Proofs

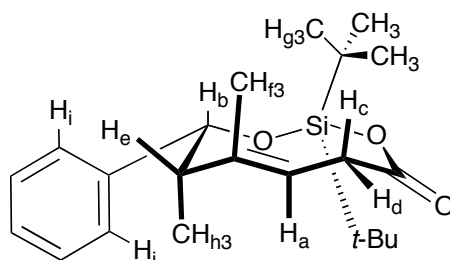
nOe Experiments:



Cyclononene **5**:

H_a irradiated:	H_d (7.5%)	H_b irradiated:	H_f (5.9%)	H_e irradiated:	H_a (15.9%)	H_f irradiated:	H_b (2.6%)
	H_e (17.6%)		H_g (7.3%)		H_h (5.5%)		H_c (3.7%)
			H_h (2.9%)		H_i (6.7%)		H_h (2.6%)
			H_i (14.3%)				

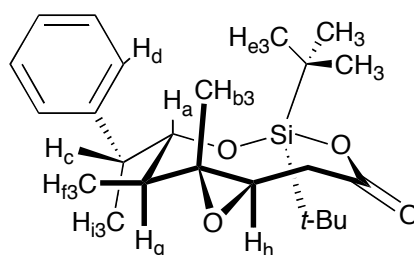
The stereochemistry of cyclononene **5** reveals that the addition of vinyl oxasilacyclopentene **3** to benzaldehyde occurred in a closed chair-like transition state. Lack of nOe correlation between H_a and H_f reveal that the alkene is *trans*.



Cyclononene 7:

H_a irradiated:	H_d (7.1%) H_h (10.1%)	H_b irradiated:	H_e (8.6%) H_f (7.6%) H_g (10.2%) H_i (12.1%)	H_c irradiated:	H_b (7.9%) H_f (6.8%) H_h (6.1%) H_i (6.7%)	H_f irradiated:	H_b (2.9%) H_c (3.8%) H_e (3.5%)
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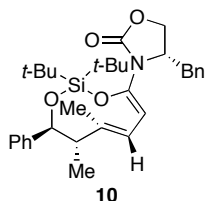
The stereochemistry of cyclononene **7** reveals that the addition of vinyl oxasilacyclopentene from *trans*-dienoate **6** to benzaldehyde occurred in a closed chair-like transition state. Lack of nOe correlation between H_a and H_f reveal that the alkene is *trans*. Additionally lack of nOe correlation between H_f and H_h reveal that the two methyl groups are *trans* to one another as they were in the dienophile **6**.

Epoxide **23'**:

H_a irradiated:	H_b (9.8%) H_c (9.0%) H_d (10.9%) H_e (9.5%) H_f (3.2%)	H_f irradiated:	H_a (5.4%) H_b (11.5%) H_c (16.7%) H_g (12.4%)	H_g irradiated:	H_f (6.3%) H_h (19.1%) H_i (7.7%)
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The stereochemistry of epoxide **23'** indicates that the epoxidation occurred on the outside face of the alkene. Lack of nOe correlation between H_b and H_h indicate that they are *trans* to each other.

VI. X-Ray Crystallography

A. Silacycle **10**

X-ray Data Collection, Structure Solution and Refinement for **10**.

A colorless crystal of approximate dimensions 0.17 x 0.32 x 0.33 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2¹ program package was used to determine the unit-cell parameters and for data collection (25 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT² and SADABS³ to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL⁴ program. There

were no systematic absences. The noncentrosymmetric triclinic space group *P1* was assigned and later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors⁵ for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There were two molecules of the formula-unit present ($Z = 2$).

At convergence, $wR2 = 0.1037$ and $Goof = 1.032$ for 701 variables refined against 11858 data (0.80\AA), $R1 = 0.0391$ for those 11124 data with $I > 2.0\sigma(I)$. The absolute structure was assigned by refinement of the Flack parameter⁶

References.

1. APEX2 Version 2.2-0 Bruker AXS, Inc.; Madison, WI 2007.
 2. SAINT Version 7.46a, Bruker AXS, Inc.; Madison, WI 2007.
 3. Sheldrick, G. M. SADABS, Version 2008/1, Bruker AXS, Inc.; Madison, WI 2008.
 4. Sheldrick, G. M. SHELXTL, Version 2008/4, Bruker AXS, Inc.; Madison, WI 2008.
 5. International Tables for X-Ray Crystallography 1992, Vol. C., Dordrecht: Kluwer Academic Publishers
 6. Flack, H. D. Acta. Cryst., A39, 876-881, 1983.
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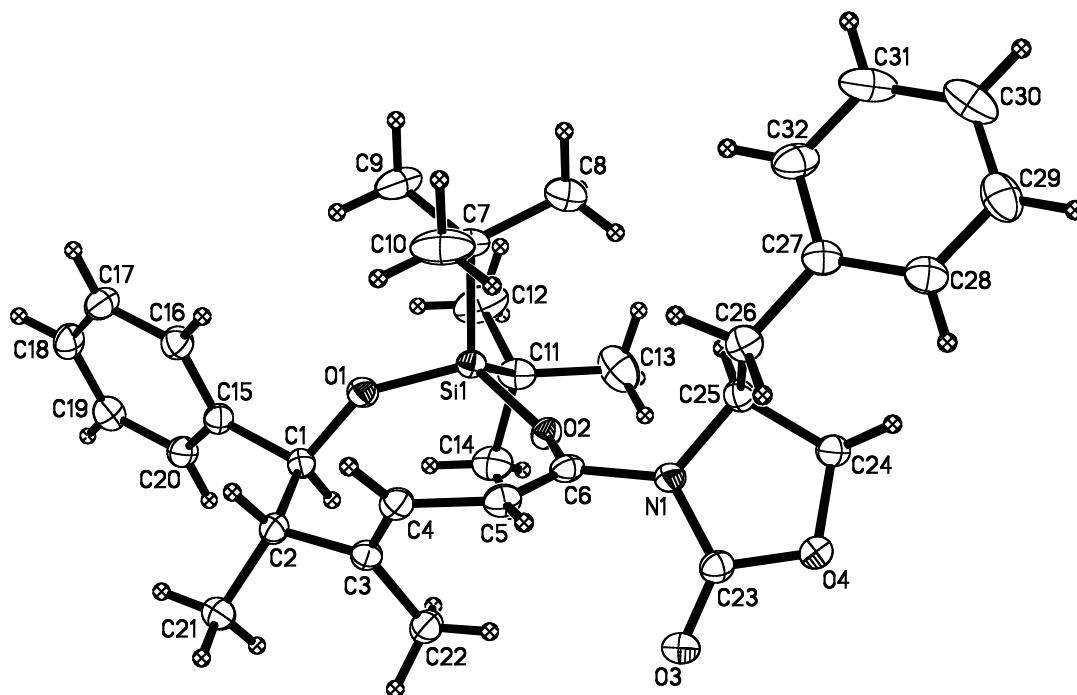
Definitions:

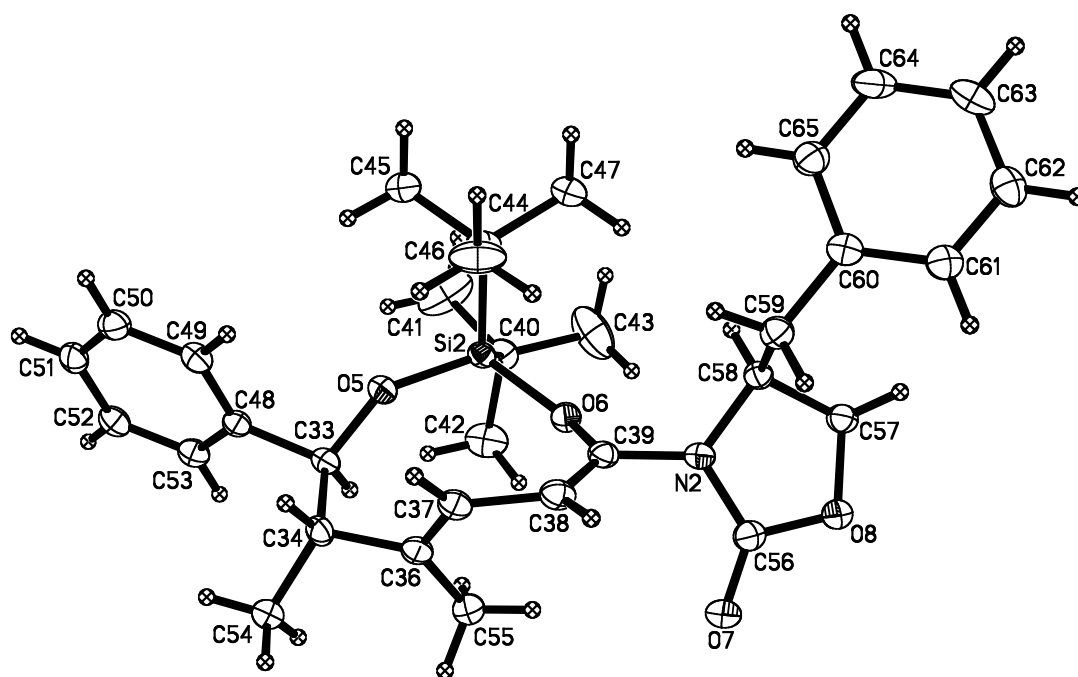
$$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$$

$$R1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$$

Goof = S = $[\Sigma[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

The thermal ellipsoid plot is shown at the 50% probability level.



Table 1. Crystal data and structure refinement for **10**.

Identification code	10 (Christian Ventocilla)	
Empirical formula	C ₃₂ H ₄₃ N O ₄ Si	
Formula weight	533.76	
Temperature	143(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	<i>P</i> 1	
Unit cell dimensions	a = 9.0489(9) Å	∠ = 96.5484(12)°.
	b = 11.8543(12) Å	∠ = 99.1573(12)°.
	c = 14.1652(14) Å	∠ = 90.8419(12)°.
Volume	1489.5(3) Å ³	
Z	2	
Density (calculated)	1.190 Mg/m ³	
Absorption coefficient	0.115 mm ⁻¹	
F(000)	576	
Crystal color	colorless	

Crystal size	0.33 x 0.32 x 0.17 mm ³
Theta range for data collection	1.47 to 26.37°
Index ranges	-11 ≤ <i>h</i> ≤ 11, -14 ≤ <i>k</i> ≤ 14, -17 ≤ <i>l</i> ≤ 17
Reflections collected	15959
Independent reflections	11858 [R(int) = 0.0193]
Completeness to theta = 25.50°	99.6 %
Absorption correction	Numerical
Max. and min. transmission	0.9803 and 0.9636
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11858 / 3 / 701
Goodness-of-fit on F ²	1.032
Final R indices [I > 2σ(I) = 11124 data]	R1 = 0.0391, wR2 = 0.1009
R indices (all data, 0.80 Å)	R1 = 0.0424, wR2 = 0.1037
Absolute structure parameter	0.05(7)
Largest diff. peak and hole	0.455 and -0.219 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **10**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	5602(1)	614(1)	9826(1)	17(1)
Si(2)	13580(1)	-3633(1)	15033(1)	17(1)
O(1)	5816(2)	1983(1)	10083(1)	21(1)
O(2)	6208(2)	-165(1)	10713(1)	19(1)
O(3)	7486(2)	-1295(1)	13121(1)	30(1)
O(4)	7361(2)	-3023(1)	12267(1)	23(1)
O(5)	13344(2)	-2339(1)	14776(1)	20(1)
O(6)	12987(2)	-4681(1)	14152(1)	20(1)
O(7)	11676(2)	-6503(1)	11729(1)	29(1)
O(8)	11813(2)	-7992(1)	12586(1)	22(1)
N(1)	7544(2)	-1524(1)	11480(1)	21(1)
N(2)	11667(2)	-6282(2)	13381(1)	22(1)
C(1)	5372(2)	2918(2)	10693(1)	20(1)
C(2)	6642(2)	3243(2)	11567(2)	20(1)
C(3)	7113(2)	2153(2)	11971(1)	20(1)
C(4)	8282(2)	1617(2)	11686(1)	20(1)
C(5)	8518(2)	401(2)	11762(2)	22(1)
C(6)	7489(2)	-366(2)	11313(1)	19(1)
C(15)	5051(2)	3896(2)	10101(2)	20(1)
C(16)	5998(2)	4148(2)	9465(2)	24(1)
C(17)	5743(3)	5053(2)	8934(2)	28(1)
C(18)	4527(3)	5731(2)	9042(2)	27(1)
C(19)	3565(2)	5491(2)	9664(2)	25(1)
C(20)	3827(2)	4574(2)	10192(2)	23(1)
C(21)	6118(3)	4134(2)	12305(2)	26(1)
C(22)	6087(2)	1661(2)	12563(2)	24(1)
C(11)	3550(2)	143(2)	9547(2)	24(1)
C(14)	2724(3)	685(2)	10346(2)	31(1)
C(13)	3360(3)	-1158(2)	9532(2)	41(1)
C(12)	2796(3)	475(3)	8584(2)	45(1)
C(7)	6762(2)	325(2)	8827(2)	22(1)

C(10)	8416(3)	590(3)	9240(2)	43(1)
C(9)	6310(3)	1093(2)	8041(2)	36(1)
C(8)	6589(3)	-909(2)	8364(2)	42(1)
C(23)	7465(2)	-1872(2)	12360(2)	21(1)
C(24)	7127(2)	-3448(2)	11252(2)	22(1)
C(25)	7684(2)	-2485(2)	10754(2)	20(1)
C(26)	9317(2)	-2592(2)	10585(2)	23(1)
C(27)	9526(2)	-3605(2)	9877(2)	23(1)
C(28)	9896(2)	-4653(2)	10195(2)	26(1)
C(29)	10006(3)	-5607(2)	9549(2)	34(1)
C(30)	9762(3)	-5517(2)	8569(2)	41(1)
C(31)	9433(3)	-4484(3)	8244(2)	40(1)
C(32)	9315(3)	-3530(2)	8888(2)	31(1)
C(33)	13797(2)	-1570(2)	14162(1)	19(1)
C(34)	12539(2)	-1519(2)	13282(2)	20(1)
C(36)	12081(2)	-2735(2)	12882(1)	21(1)
C(37)	10912(2)	-3221(2)	13163(2)	22(1)
C(38)	10683(2)	-4464(2)	13087(2)	22(1)
C(39)	11718(2)	-5084(2)	13547(1)	20(1)
C(48)	14125(2)	-415(2)	14748(1)	19(1)
C(49)	13158(2)	11(2)	15369(2)	22(1)
C(50)	13427(2)	1072(2)	15887(2)	26(1)
C(51)	14665(3)	1733(2)	15799(2)	25(1)
C(52)	15643(2)	1317(2)	15184(2)	24(1)
C(53)	15368(2)	246(2)	14666(2)	22(1)
C(54)	13074(3)	-815(2)	12548(2)	26(1)
C(55)	13119(2)	-3360(2)	12291(2)	25(1)
C(44)	12415(2)	-3688(2)	16028(2)	22(1)
C(47)	12597(3)	-4803(2)	16487(2)	32(1)
C(46)	10759(3)	-3589(3)	15603(2)	38(1)
C(45)	12836(3)	-2689(2)	16822(2)	30(1)
C(40)	15641(2)	-3939(2)	15312(2)	24(1)
C(43)	15894(3)	-5197(3)	15451(3)	52(1)
C(42)	16424(3)	-3696(2)	14470(2)	34(1)
C(41)	16398(3)	-3189(3)	16215(2)	51(1)
C(56)	11714(2)	-6870(2)	12491(2)	22(1)

C(57)	12066(2)	-8138(2)	13599(2)	21(1)
C(58)	11522(2)	-7044(2)	14106(1)	19(1)
C(59)	9893(2)	-7132(2)	14282(2)	22(1)
C(60)	9667(2)	-7968(2)	14979(2)	22(1)
C(61)	9288(2)	-9104(2)	14650(2)	24(1)
C(62)	9151(2)	-9891(2)	15286(2)	28(1)
C(63)	9388(3)	-9547(2)	16268(2)	32(1)
C(64)	9730(3)	-8415(2)	16607(2)	32(1)
C(65)	9870(2)	-7630(2)	15970(2)	26(1)

Table 3. Bond lengths [Å] and angles [°] for **10**.

Si(1)-O(1)	1.6246(15)
Si(1)-O(2)	1.6719(14)
Si(1)-C(7)	1.896(2)
Si(1)-C(11)	1.898(2)
Si(2)-O(5)	1.6260(15)
Si(2)-O(6)	1.6740(15)
Si(2)-C(40)	1.894(2)
Si(2)-C(44)	1.896(2)
O(1)-C(1)	1.428(2)
O(2)-C(6)	1.365(2)
O(3)-C(23)	1.207(3)
O(4)-C(23)	1.356(2)
O(4)-C(24)	1.449(2)
O(5)-C(33)	1.428(2)
O(6)-C(39)	1.363(2)
O(7)-C(56)	1.205(3)
O(8)-C(56)	1.355(3)
O(8)-C(57)	1.447(2)
N(1)-C(23)	1.368(3)
N(1)-C(6)	1.419(3)
N(1)-C(25)	1.466(2)
N(2)-C(56)	1.376(3)
N(2)-C(39)	1.412(3)
N(2)-C(58)	1.463(2)
C(1)-C(15)	1.512(3)
C(1)-C(2)	1.558(3)
C(2)-C(3)	1.512(3)
C(2)-C(21)	1.534(3)
C(3)-C(4)	1.335(3)
C(3)-C(22)	1.500(3)
C(4)-C(5)	1.474(3)
C(5)-C(6)	1.324(3)
C(15)-C(16)	1.391(3)
C(15)-C(20)	1.393(3)

C(16)-C(17)	1.380(3)
C(17)-C(18)	1.390(3)
C(18)-C(19)	1.382(3)
C(19)-C(20)	1.391(3)
C(11)-C(12)	1.521(3)
C(11)-C(14)	1.540(3)
C(11)-C(13)	1.547(3)
C(7)-C(9)	1.527(3)
C(7)-C(8)	1.528(3)
C(7)-C(10)	1.532(3)
C(24)-C(25)	1.528(3)
C(25)-C(26)	1.539(3)
C(26)-C(27)	1.508(3)
C(27)-C(32)	1.397(3)
C(27)-C(28)	1.397(3)
C(28)-C(29)	1.386(3)
C(29)-C(30)	1.388(4)
C(30)-C(31)	1.376(4)
C(31)-C(32)	1.386(4)
C(33)-C(48)	1.517(3)
C(33)-C(34)	1.555(3)
C(34)-C(36)	1.514(3)
C(34)-C(54)	1.536(3)
C(36)-C(37)	1.333(3)
C(36)-C(55)	1.503(3)
C(37)-C(38)	1.474(3)
C(38)-C(39)	1.333(3)
C(48)-C(53)	1.389(3)
C(48)-C(49)	1.397(3)
C(49)-C(50)	1.380(3)
C(50)-C(51)	1.388(3)
C(51)-C(52)	1.395(3)
C(52)-C(53)	1.390(3)
C(44)-C(46)	1.535(3)
C(44)-C(45)	1.536(3)
C(44)-C(47)	1.539(3)

C(40)-C(41)	1.529(3)
C(40)-C(42)	1.533(3)
C(40)-C(43)	1.542(3)
C(57)-C(58)	1.535(3)
C(58)-C(59)	1.538(3)
C(59)-C(60)	1.510(3)
C(60)-C(61)	1.393(3)
C(60)-C(65)	1.397(3)
C(61)-C(62)	1.386(3)
C(62)-C(63)	1.386(4)
C(63)-C(64)	1.386(4)
C(64)-C(65)	1.386(3)

O(1)-Si(1)-O(2)	116.47(7)
O(1)-Si(1)-C(7)	101.86(9)
O(2)-Si(1)-C(7)	109.46(8)
O(1)-Si(1)-C(11)	111.87(9)
O(2)-Si(1)-C(11)	100.46(9)
C(7)-Si(1)-C(11)	117.44(10)
O(5)-Si(2)-O(6)	117.00(8)
O(5)-Si(2)-C(40)	111.01(9)
O(6)-Si(2)-C(40)	100.99(9)
O(5)-Si(2)-C(44)	101.72(9)
O(6)-Si(2)-C(44)	108.98(9)
C(40)-Si(2)-C(44)	117.91(10)
C(1)-O(1)-Si(1)	142.11(13)
C(6)-O(2)-Si(1)	140.41(13)
C(23)-O(4)-C(24)	108.86(15)
C(33)-O(5)-Si(2)	141.07(13)
C(39)-O(6)-Si(2)	140.59(13)
C(56)-O(8)-C(57)	109.16(15)
C(23)-N(1)-C(6)	122.91(17)
C(23)-N(1)-C(25)	111.80(16)
C(6)-N(1)-C(25)	125.29(16)
C(56)-N(2)-C(39)	122.85(17)
C(56)-N(2)-C(58)	111.96(17)

C(39)-N(2)-C(58)	125.17(16)
O(1)-C(1)-C(15)	107.95(16)
O(1)-C(1)-C(2)	109.59(15)
C(15)-C(1)-C(2)	111.37(16)
C(3)-C(2)-C(21)	113.57(17)
C(3)-C(2)-C(1)	106.97(16)
C(21)-C(2)-C(1)	110.81(17)
C(4)-C(3)-C(22)	123.83(19)
C(4)-C(3)-C(2)	119.02(19)
C(22)-C(3)-C(2)	116.56(17)
C(3)-C(4)-C(5)	122.59(19)
C(6)-C(5)-C(4)	119.82(18)
C(5)-C(6)-O(2)	126.59(18)
C(5)-C(6)-N(1)	122.08(18)
O(2)-C(6)-N(1)	111.10(17)
C(16)-C(15)-C(20)	118.66(19)
C(16)-C(15)-C(1)	120.27(18)
C(20)-C(15)-C(1)	121.06(18)
C(17)-C(16)-C(15)	121.1(2)
C(16)-C(17)-C(18)	119.6(2)
C(19)-C(18)-C(17)	120.3(2)
C(18)-C(19)-C(20)	119.7(2)
C(19)-C(20)-C(15)	120.6(2)
C(12)-C(11)-C(14)	109.0(2)
C(12)-C(11)-C(13)	108.7(2)
C(14)-C(11)-C(13)	106.40(19)
C(12)-C(11)-Si(1)	111.87(16)
C(14)-C(11)-Si(1)	109.63(15)
C(13)-C(11)-Si(1)	111.06(15)
C(9)-C(7)-C(8)	108.3(2)
C(9)-C(7)-C(10)	107.7(2)
C(8)-C(7)-C(10)	108.8(2)
C(9)-C(7)-Si(1)	110.51(15)
C(8)-C(7)-Si(1)	112.30(16)
C(10)-C(7)-Si(1)	109.07(15)
O(3)-C(23)-O(4)	122.57(19)

O(3)-C(23)-N(1)	128.3(2)
O(4)-C(23)-N(1)	109.12(17)
O(4)-C(24)-C(25)	105.08(16)
N(1)-C(25)-C(24)	99.40(15)
N(1)-C(25)-C(26)	110.85(16)
C(24)-C(25)-C(26)	113.85(16)
C(27)-C(26)-C(25)	112.68(17)
C(32)-C(27)-C(28)	118.2(2)
C(32)-C(27)-C(26)	121.1(2)
C(28)-C(27)-C(26)	120.62(19)
C(29)-C(28)-C(27)	121.3(2)
C(28)-C(29)-C(30)	119.4(2)
C(31)-C(30)-C(29)	120.1(2)
C(30)-C(31)-C(32)	120.6(2)
C(31)-C(32)-C(27)	120.4(2)
O(5)-C(33)-C(48)	108.04(16)
O(5)-C(33)-C(34)	109.63(16)
C(48)-C(33)-C(34)	111.64(16)
C(36)-C(34)-C(54)	113.86(17)
C(36)-C(34)-C(33)	106.85(16)
C(54)-C(34)-C(33)	110.64(17)
C(37)-C(36)-C(55)	124.16(19)
C(37)-C(36)-C(34)	118.91(19)
C(55)-C(36)-C(34)	116.42(18)
C(36)-C(37)-C(38)	122.47(19)
C(39)-C(38)-C(37)	119.70(19)
C(38)-C(39)-O(6)	126.42(19)
C(38)-C(39)-N(2)	121.80(18)
O(6)-C(39)-N(2)	111.57(17)
C(53)-C(48)-C(49)	118.77(19)
C(53)-C(48)-C(33)	120.96(18)
C(49)-C(48)-C(33)	120.25(18)
C(50)-C(49)-C(48)	120.67(19)
C(49)-C(50)-C(51)	120.4(2)
C(50)-C(51)-C(52)	119.6(2)
C(53)-C(52)-C(51)	119.66(19)

C(48)-C(53)-C(52)	120.89(19)
C(46)-C(44)-C(45)	107.59(19)
C(46)-C(44)-C(47)	108.54(19)
C(45)-C(44)-C(47)	108.59(18)
C(46)-C(44)-Si(2)	108.80(15)
C(45)-C(44)-Si(2)	111.10(15)
C(47)-C(44)-Si(2)	112.08(15)
C(41)-C(40)-C(42)	108.2(2)
C(41)-C(40)-C(43)	109.2(2)
C(42)-C(40)-C(43)	106.6(2)
C(41)-C(40)-Si(2)	110.84(16)
C(42)-C(40)-Si(2)	109.89(15)
C(43)-C(40)-Si(2)	111.93(16)
O(7)-C(56)-O(8)	122.75(19)
O(7)-C(56)-N(2)	128.5(2)
O(8)-C(56)-N(2)	108.74(17)
O(8)-C(57)-C(58)	105.04(16)
N(2)-C(58)-C(57)	99.10(15)
N(2)-C(58)-C(59)	111.01(16)
C(57)-C(58)-C(59)	113.92(16)
C(60)-C(59)-C(58)	113.00(17)
C(61)-C(60)-C(65)	118.4(2)
C(61)-C(60)-C(59)	120.67(19)
C(65)-C(60)-C(59)	120.95(19)
C(62)-C(61)-C(60)	121.2(2)
C(63)-C(62)-C(61)	119.7(2)
C(64)-C(63)-C(62)	119.9(2)
C(63)-C(64)-C(65)	120.3(2)
C(64)-C(65)-C(60)	120.5(2)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **10**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Si(1)	15(1)	19(1)	15(1)	2(1)	0(1)	2(1)
Si(2)	16(1)	19(1)	15(1)	4(1)	0(1)	0(1)
O(1)	24(1)	20(1)	18(1)	2(1)	2(1)	3(1)
O(2)	19(1)	20(1)	19(1)	5(1)	0(1)	0(1)
O(3)	43(1)	27(1)	19(1)	2(1)	8(1)	3(1)
O(4)	26(1)	22(1)	20(1)	4(1)	4(1)	1(1)
O(5)	23(1)	20(1)	19(1)	5(1)	3(1)	1(1)
O(6)	20(1)	21(1)	19(1)	3(1)	-1(1)	1(1)
O(7)	41(1)	29(1)	19(1)	5(1)	7(1)	-1(1)
O(8)	26(1)	22(1)	20(1)	2(1)	5(1)	1(1)
N(1)	28(1)	19(1)	15(1)	3(1)	3(1)	4(1)
N(2)	28(1)	22(1)	15(1)	3(1)	4(1)	-1(1)
C(1)	22(1)	17(1)	19(1)	2(1)	3(1)	0(1)
C(2)	24(1)	18(1)	19(1)	4(1)	2(1)	-1(1)
C(3)	22(1)	21(1)	16(1)	2(1)	-1(1)	-2(1)
C(4)	19(1)	24(1)	17(1)	3(1)	-2(1)	-3(1)
C(5)	18(1)	28(1)	18(1)	5(1)	1(1)	3(1)
C(6)	21(1)	23(1)	15(1)	5(1)	4(1)	7(1)
C(15)	22(1)	20(1)	18(1)	4(1)	-2(1)	0(1)
C(16)	24(1)	23(1)	26(1)	3(1)	6(1)	1(1)
C(17)	34(1)	30(1)	23(1)	7(1)	6(1)	-3(1)
C(18)	33(1)	23(1)	24(1)	8(1)	-4(1)	0(1)
C(19)	24(1)	24(1)	26(1)	2(1)	-2(1)	5(1)
C(20)	23(1)	23(1)	22(1)	4(1)	4(1)	2(1)
C(21)	33(1)	23(1)	22(1)	1(1)	3(1)	1(1)
C(22)	28(1)	24(1)	24(1)	6(1)	6(1)	2(1)
C(11)	15(1)	34(1)	21(1)	1(1)	0(1)	-1(1)
C(14)	20(1)	42(1)	31(1)	1(1)	8(1)	-5(1)
C(13)	27(1)	37(1)	54(2)	-9(1)	6(1)	-8(1)
C(12)	25(1)	80(2)	30(1)	16(1)	-5(1)	-2(1)
C(7)	19(1)	30(1)	16(1)	2(1)	4(1)	3(1)

C(10)	21(1)	81(2)	27(1)	0(1)	7(1)	-1(1)
C(9)	36(1)	50(2)	26(1)	16(1)	13(1)	14(1)
C(8)	57(2)	36(1)	36(1)	-1(1)	25(1)	3(1)
C(23)	20(1)	24(1)	20(1)	4(1)	3(1)	3(1)
C(24)	23(1)	23(1)	20(1)	2(1)	5(1)	1(1)
C(25)	21(1)	19(1)	18(1)	1(1)	1(1)	2(1)
C(26)	22(1)	25(1)	23(1)	2(1)	2(1)	-1(1)
C(27)	17(1)	29(1)	22(1)	2(1)	4(1)	2(1)
C(28)	20(1)	32(1)	25(1)	2(1)	5(1)	3(1)
C(29)	26(1)	29(1)	47(2)	-1(1)	9(1)	4(1)
C(30)	33(1)	45(2)	41(2)	-14(1)	10(1)	6(1)
C(31)	34(1)	62(2)	23(1)	-2(1)	8(1)	11(1)
C(32)	27(1)	44(1)	26(1)	10(1)	10(1)	11(1)
C(33)	21(1)	20(1)	18(1)	6(1)	4(1)	1(1)
C(34)	23(1)	18(1)	20(1)	5(1)	0(1)	3(1)
C(36)	23(1)	22(1)	16(1)	5(1)	-2(1)	3(1)
C(37)	22(1)	25(1)	18(1)	6(1)	-3(1)	4(1)
C(38)	21(1)	28(1)	18(1)	4(1)	0(1)	-2(1)
C(39)	21(1)	22(1)	16(1)	3(1)	3(1)	-5(1)
C(48)	22(1)	20(1)	16(1)	5(1)	-1(1)	4(1)
C(49)	20(1)	24(1)	24(1)	8(1)	5(1)	3(1)
C(50)	28(1)	28(1)	22(1)	6(1)	6(1)	9(1)
C(51)	32(1)	21(1)	20(1)	4(1)	-4(1)	2(1)
C(52)	20(1)	26(1)	25(1)	8(1)	2(1)	-2(1)
C(53)	18(1)	26(1)	21(1)	6(1)	2(1)	1(1)
C(54)	34(1)	24(1)	21(1)	5(1)	5(1)	3(1)
C(55)	28(1)	24(1)	23(1)	2(1)	6(1)	0(1)
C(44)	24(1)	29(1)	15(1)	4(1)	4(1)	-2(1)
C(47)	45(1)	30(1)	25(1)	6(1)	12(1)	-3(1)
C(46)	21(1)	70(2)	24(1)	10(1)	6(1)	3(1)
C(45)	40(1)	29(1)	22(1)	2(1)	10(1)	-2(1)
C(40)	19(1)	26(1)	24(1)	5(1)	-1(1)	2(1)
C(43)	32(1)	46(2)	84(2)	35(2)	9(1)	14(1)
C(42)	20(1)	50(2)	34(1)	11(1)	7(1)	11(1)
C(41)	22(1)	84(2)	37(2)	-19(2)	-6(1)	5(1)
C(56)	20(1)	25(1)	20(1)	1(1)	4(1)	-3(1)

C(57)	23(1)	23(1)	19(1)	4(1)	3(1)	1(1)
C(58)	22(1)	19(1)	16(1)	3(1)	0(1)	-2(1)
C(59)	22(1)	23(1)	21(1)	3(1)	2(1)	3(1)
C(60)	18(1)	27(1)	22(1)	5(1)	4(1)	3(1)
C(61)	19(1)	29(1)	24(1)	3(1)	4(1)	-1(1)
C(62)	20(1)	28(1)	37(1)	6(1)	8(1)	-1(1)
C(63)	27(1)	41(1)	32(1)	17(1)	10(1)	0(1)
C(64)	32(1)	46(1)	20(1)	6(1)	7(1)	-5(1)
C(65)	24(1)	29(1)	25(1)	1(1)	6(1)	-4(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **10**.

	x	y	z	U(eq)
H(1A)	4441	2694	10932	23
H(2A)	7514	3575	11327	25
H(4A)	8989	2035	11424	25
H(5A)	9405	168	12133	26
H(16A)	6835	3689	9394	29
H(17A)	6394	5211	8498	34
H(18A)	4356	6363	8686	33
H(19A)	2727	5951	9730	30
H(20A)	3164	4409	10619	27
H(21A)	6924	4313	12854	39
H(21B)	5236	3833	12526	39
H(21C)	5860	4825	12004	39
H(22A)	6412	902	12698	37
H(22B)	5062	1605	12208	37
H(22C)	6118	2153	13171	37
H(14A)	1710	346	10259	46
H(14B)	2665	1505	10313	46
H(14C)	3271	550	10976	46
H(13A)	2292	-1373	9429	61
H(13B)	3845	-1383	10149	61
H(13C)	3825	-1543	9010	61
H(12A)	1728	261	8484	68
H(12B)	3259	79	8065	68
H(12C)	2917	1297	8582	68
H(10A)	9018	468	8723	65
H(10B)	8746	89	9732	65
H(10C)	8542	1384	9531	65
H(9A)	6950	957	7545	53
H(9B)	6429	1889	8323	53
H(9C)	5262	925	7750	53

H(8A)	7250	-1030	7879	62
H(8B)	5548	-1072	8056	62
H(8C)	6860	-1416	8860	62
H(24A)	6052	-3631	11012	26
H(24B)	7703	-4140	11137	26
H(25A)	7002	-2407	10137	24
H(26A)	9637	-1892	10342	28
H(26B)	9967	-2658	11207	28
H(28A)	10075	-4714	10866	31
H(29A)	10246	-6317	9776	41
H(30A)	9822	-6169	8121	49
H(31A)	9286	-4424	7573	48
H(32A)	9090	-2821	8655	38
H(33A)	14730	-1844	13928	23
H(34A)	11660	-1144	13515	24
H(37A)	10201	-2748	13422	26
H(38A)	9801	-4821	12711	27
H(49A)	12306	-434	15435	26
H(50A)	12760	1352	16307	31
H(51A)	14845	2464	16155	30
H(52A)	16494	1763	15120	28
H(53A)	16039	-38	14251	26
H(54A)	12279	-813	11991	39
H(54B)	13969	-1149	12338	39
H(54C)	13315	-34	12848	39
H(55A)	12805	-4165	12159	37
H(55B)	14143	-3286	12647	37
H(55C)	13084	-3035	11682	37
H(47A)	11912	-4826	16956	48
H(47B)	13631	-4845	16813	48
H(47C)	12364	-5449	15985	48
H(46A)	10148	-3599	16115	57
H(46B)	10448	-4230	15106	57
H(46C)	10622	-2875	15318	57
H(45A)	12206	-2729	17321	45
H(45B)	12679	-1971	16545	45

H(45C)	13891	-2729	17108	45
H(43A)	16970	-5336	15538	77
H(43B)	15385	-5682	14881	77
H(43C)	15489	-5374	16020	77
H(42A)	17460	-3941	14584	51
H(42B)	16420	-2879	14415	51
H(42C)	15893	-4111	13872	51
H(41A)	17477	-3314	16315	76
H(41B)	15978	-3385	16774	76
H(41C)	16223	-2390	16135	76
H(57A)	13142	-8236	13831	26
H(57B)	11490	-8810	13718	26
H(58A)	12212	-6789	14721	23
H(59A)	9589	-6373	14537	27
H(59B)	9234	-7365	13660	27
H(61A)	9121	-9343	13977	29
H(62A)	8896	-10663	15050	33
H(63A)	9316	-10086	16707	38
H(64A)	9868	-8176	17279	39
H(65A)	10106	-6856	16209	31

Table 6. Torsion angles [°] for **10**.

O(2)-Si(1)-O(1)-C(1)	-62.5(2)
C(7)-Si(1)-O(1)-C(1)	178.5(2)
C(11)-Si(1)-O(1)-C(1)	52.2(2)
O(1)-Si(1)-O(2)-C(6)	-59.5(2)
C(7)-Si(1)-O(2)-C(6)	55.3(2)
C(11)-Si(1)-O(2)-C(6)	179.5(2)
O(6)-Si(2)-O(5)-C(33)	-63.1(2)
C(40)-Si(2)-O(5)-C(33)	52.0(2)
C(44)-Si(2)-O(5)-C(33)	178.3(2)
O(5)-Si(2)-O(6)-C(39)	-58.2(2)
C(40)-Si(2)-O(6)-C(39)	-178.8(2)
C(44)-Si(2)-O(6)-C(39)	56.4(2)
Si(1)-O(1)-C(1)-C(15)	-138.61(18)
Si(1)-O(1)-C(1)-C(2)	99.9(2)
O(1)-C(1)-C(2)-C(3)	-48.1(2)
C(15)-C(1)-C(2)-C(3)	-167.43(16)
O(1)-C(1)-C(2)-C(21)	-172.33(16)
C(15)-C(1)-C(2)-C(21)	68.3(2)
C(21)-C(2)-C(3)-C(4)	-142.4(2)
C(1)-C(2)-C(3)-C(4)	95.1(2)
C(21)-C(2)-C(3)-C(22)	46.1(2)
C(1)-C(2)-C(3)-C(22)	-76.5(2)
C(22)-C(3)-C(4)-C(5)	12.2(3)
C(2)-C(3)-C(4)-C(5)	-158.71(19)
C(3)-C(4)-C(5)-C(6)	59.4(3)
C(4)-C(5)-C(6)-O(2)	4.1(3)
C(4)-C(5)-C(6)-N(1)	-169.99(18)
Si(1)-O(2)-C(6)-C(5)	41.7(3)
Si(1)-O(2)-C(6)-N(1)	-143.70(17)
C(23)-N(1)-C(6)-C(5)	62.0(3)
C(25)-N(1)-C(6)-C(5)	-118.2(2)
C(23)-N(1)-C(6)-O(2)	-112.9(2)
C(25)-N(1)-C(6)-O(2)	66.9(2)
O(1)-C(1)-C(15)-C(16)	-42.5(2)

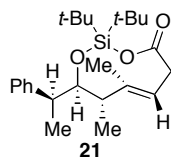
C(2)-C(1)-C(15)-C(16)	77.9(2)
O(1)-C(1)-C(15)-C(20)	138.79(19)
C(2)-C(1)-C(15)-C(20)	-100.9(2)
C(20)-C(15)-C(16)-C(17)	0.3(3)
C(1)-C(15)-C(16)-C(17)	-178.53(19)
C(15)-C(16)-C(17)-C(18)	0.5(3)
C(16)-C(17)-C(18)-C(19)	-1.0(3)
C(17)-C(18)-C(19)-C(20)	0.7(3)
C(18)-C(19)-C(20)-C(15)	0.1(3)
C(16)-C(15)-C(20)-C(19)	-0.6(3)
C(1)-C(15)-C(20)-C(19)	178.22(19)
O(1)-Si(1)-C(11)-C(12)	71.2(2)
O(2)-Si(1)-C(11)-C(12)	-164.53(18)
C(7)-Si(1)-C(11)-C(12)	-46.0(2)
O(1)-Si(1)-C(11)-C(14)	-49.81(18)
O(2)-Si(1)-C(11)-C(14)	74.42(17)
C(7)-Si(1)-C(11)-C(14)	-167.05(15)
O(1)-Si(1)-C(11)-C(13)	-167.11(16)
O(2)-Si(1)-C(11)-C(13)	-42.88(18)
C(7)-Si(1)-C(11)-C(13)	75.65(19)
O(1)-Si(1)-C(7)-C(9)	-51.83(18)
O(2)-Si(1)-C(7)-C(9)	-175.69(15)
C(11)-Si(1)-C(7)-C(9)	70.71(19)
O(1)-Si(1)-C(7)-C(8)	-172.88(17)
O(2)-Si(1)-C(7)-C(8)	63.26(19)
C(11)-Si(1)-C(7)-C(8)	-50.3(2)
O(1)-Si(1)-C(7)-C(10)	66.45(19)
O(2)-Si(1)-C(7)-C(10)	-57.4(2)
C(11)-Si(1)-C(7)-C(10)	-171.02(18)
C(24)-O(4)-C(23)-O(3)	171.08(19)
C(24)-O(4)-C(23)-N(1)	-9.2(2)
C(6)-N(1)-C(23)-O(3)	-7.7(3)
C(25)-N(1)-C(23)-O(3)	172.5(2)
C(6)-N(1)-C(23)-O(4)	172.58(17)
C(25)-N(1)-C(23)-O(4)	-7.2(2)
C(23)-O(4)-C(24)-C(25)	21.0(2)

C(23)-N(1)-C(25)-C(24)	19.0(2)
C(6)-N(1)-C(25)-C(24)	-160.83(18)
C(23)-N(1)-C(25)-C(26)	-101.2(2)
C(6)-N(1)-C(25)-C(26)	79.1(2)
O(4)-C(24)-C(25)-N(1)	-23.05(18)
O(4)-C(24)-C(25)-C(26)	94.83(19)
N(1)-C(25)-C(26)-C(27)	177.24(17)
C(24)-C(25)-C(26)-C(27)	66.2(2)
C(25)-C(26)-C(27)-C(32)	87.1(2)
C(25)-C(26)-C(27)-C(28)	-91.0(2)
C(32)-C(27)-C(28)-C(29)	-2.0(3)
C(26)-C(27)-C(28)-C(29)	176.2(2)
C(27)-C(28)-C(29)-C(30)	0.8(3)
C(28)-C(29)-C(30)-C(31)	0.8(4)
C(29)-C(30)-C(31)-C(32)	-1.2(4)
C(30)-C(31)-C(32)-C(27)	-0.1(4)
C(28)-C(27)-C(32)-C(31)	1.7(3)
C(26)-C(27)-C(32)-C(31)	-176.5(2)
Si(2)-O(5)-C(33)-C(48)	-137.94(17)
Si(2)-O(5)-C(33)-C(34)	100.2(2)
O(5)-C(33)-C(34)-C(36)	-48.5(2)
C(48)-C(33)-C(34)-C(36)	-168.18(16)
O(5)-C(33)-C(34)-C(54)	-172.95(16)
C(48)-C(33)-C(34)-C(54)	67.4(2)
C(54)-C(34)-C(36)-C(37)	-142.5(2)
C(33)-C(34)-C(36)-C(37)	95.0(2)
C(54)-C(34)-C(36)-C(55)	45.4(2)
C(33)-C(34)-C(36)-C(55)	-77.0(2)
C(55)-C(36)-C(37)-C(38)	12.4(3)
C(34)-C(36)-C(37)-C(38)	-159.06(19)
C(36)-C(37)-C(38)-C(39)	59.6(3)
C(37)-C(38)-C(39)-O(6)	4.1(3)
C(37)-C(38)-C(39)-N(2)	-170.06(18)
Si(2)-O(6)-C(39)-C(38)	41.0(3)
Si(2)-O(6)-C(39)-N(2)	-144.41(17)
C(56)-N(2)-C(39)-C(38)	60.0(3)

C(58)-N(2)-C(39)-C(38)	-118.4(2)
C(56)-N(2)-C(39)-O(6)	-114.9(2)
C(58)-N(2)-C(39)-O(6)	66.7(2)
O(5)-C(33)-C(48)-C(53)	137.55(18)
C(34)-C(33)-C(48)-C(53)	-101.8(2)
O(5)-C(33)-C(48)-C(49)	-43.7(2)
C(34)-C(33)-C(48)-C(49)	76.9(2)
C(53)-C(48)-C(49)-C(50)	0.4(3)
C(33)-C(48)-C(49)-C(50)	-178.39(18)
C(48)-C(49)-C(50)-C(51)	0.0(3)
C(49)-C(50)-C(51)-C(52)	-0.3(3)
C(50)-C(51)-C(52)-C(53)	0.1(3)
C(49)-C(48)-C(53)-C(52)	-0.6(3)
C(33)-C(48)-C(53)-C(52)	178.17(18)
C(51)-C(52)-C(53)-C(48)	0.4(3)
O(5)-Si(2)-C(44)-C(46)	66.62(18)
O(6)-Si(2)-C(44)-C(46)	-57.55(18)
C(40)-Si(2)-C(44)-C(46)	-171.77(16)
O(5)-Si(2)-C(44)-C(45)	-51.65(16)
O(6)-Si(2)-C(44)-C(45)	-175.82(14)
C(40)-Si(2)-C(44)-C(45)	69.96(18)
O(5)-Si(2)-C(44)-C(47)	-173.34(15)
O(6)-Si(2)-C(44)-C(47)	62.49(17)
C(40)-Si(2)-C(44)-C(47)	-51.73(19)
O(5)-Si(2)-C(40)-C(41)	64.0(2)
O(6)-Si(2)-C(40)-C(41)	-171.30(19)
C(44)-Si(2)-C(40)-C(41)	-52.8(2)
O(5)-Si(2)-C(40)-C(42)	-55.59(18)
O(6)-Si(2)-C(40)-C(42)	69.16(17)
C(44)-Si(2)-C(40)-C(42)	-172.30(15)
O(5)-Si(2)-C(40)-C(43)	-173.85(19)
O(6)-Si(2)-C(40)-C(43)	-49.1(2)
C(44)-Si(2)-C(40)-C(43)	69.4(2)
C(57)-O(8)-C(56)-O(7)	171.29(19)
C(57)-O(8)-C(56)-N(2)	-8.8(2)
C(39)-N(2)-C(56)-O(7)	-6.8(3)

C(58)-N(2)-C(56)-O(7)	171.8(2)
C(39)-N(2)-C(56)-O(8)	173.29(17)
C(58)-N(2)-C(56)-O(8)	-8.1(2)
C(56)-O(8)-C(57)-C(58)	21.1(2)
C(56)-N(2)-C(58)-C(57)	19.8(2)
C(39)-N(2)-C(58)-C(57)	-161.68(18)
C(56)-N(2)-C(58)-C(59)	-100.3(2)
C(39)-N(2)-C(58)-C(59)	78.2(2)
O(8)-C(57)-C(58)-N(2)	-23.55(18)
O(8)-C(57)-C(58)-C(59)	94.38(19)
N(2)-C(58)-C(59)-C(60)	176.31(17)
C(57)-C(58)-C(59)-C(60)	65.5(2)
C(58)-C(59)-C(60)-C(61)	-90.3(2)
C(58)-C(59)-C(60)-C(65)	88.0(2)
C(65)-C(60)-C(61)-C(62)	-1.6(3)
C(59)-C(60)-C(61)-C(62)	176.75(18)
C(60)-C(61)-C(62)-C(63)	0.2(3)
C(61)-C(62)-C(63)-C(64)	1.3(3)
C(62)-C(63)-C(64)-C(65)	-1.5(3)
C(63)-C(64)-C(65)-C(60)	0.1(3)
C(61)-C(60)-C(65)-C(64)	1.4(3)
C(59)-C(60)-C(65)-C(64)	-176.9(2)

B. Silacycle 21



X-ray Data Collection, Structure Solution and Refinement for **21**.

A colorless crystal of approximate dimensions 0.13 x 0.21 x 0.25 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2¹ program package was used to determine the unit-cell parameters and for data collection (25 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT² and SADABS³ to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL⁴ program. There were no systematic absences nor any diffraction symmetry other than the Friedel condition. The centrosymmetric triclinic space group $P\bar{1}$ was assigned and later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors⁵ for neutral atoms were used throughout the analysis. Hydrogen atoms were located from a difference-Fourier map and refined (x,y,z and U_{iso}).

At convergence, $wR2 = 0.0931$ and $Goof = 1.043$ for 405 variables refined against 5135 data (0.78\AA), $R1 = 0.0340$ for those 4614 data with $I > 2.0\sigma(I)$.

References.

7. APEX2 Version 2008.3-0, Bruker AXS, Inc.; Madison, WI 2008.
 8. SAINT Version 7.53a, Bruker AXS, Inc.; Madison, WI 2007.
 9. Sheldrick, G. M. SADABS, Version 2007/4, Bruker AXS, Inc.; Madison, WI 2007.
 10. Sheldrick, G. M. SHELXTL, Version 2008/4, Bruker AXS, Inc.; Madison, WI 2008.
 11. International Tables for X-Ray Crystallography 1992, Vol. C., Dordrecht: Kluwer Academic Publishers.
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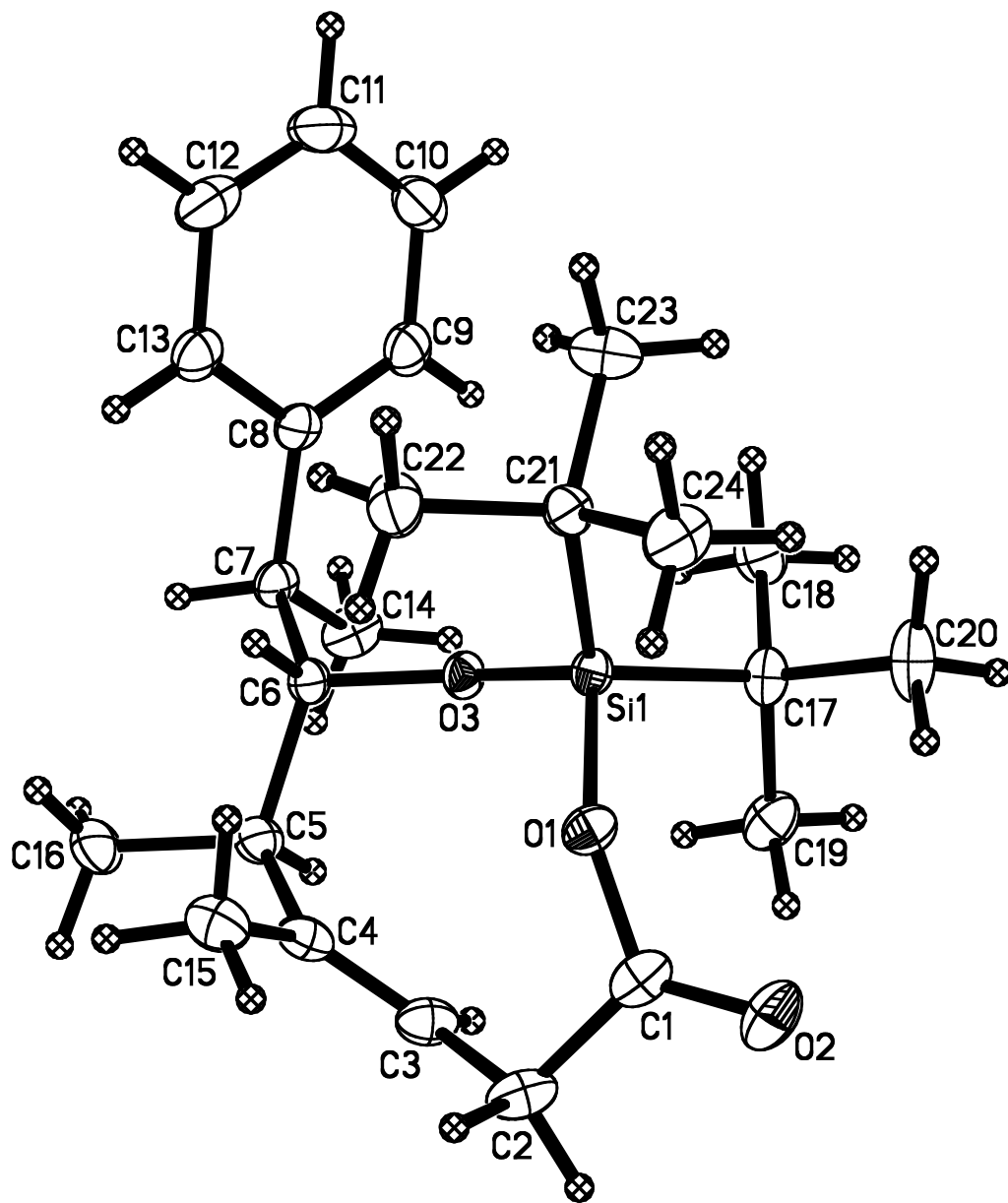
Definitions:

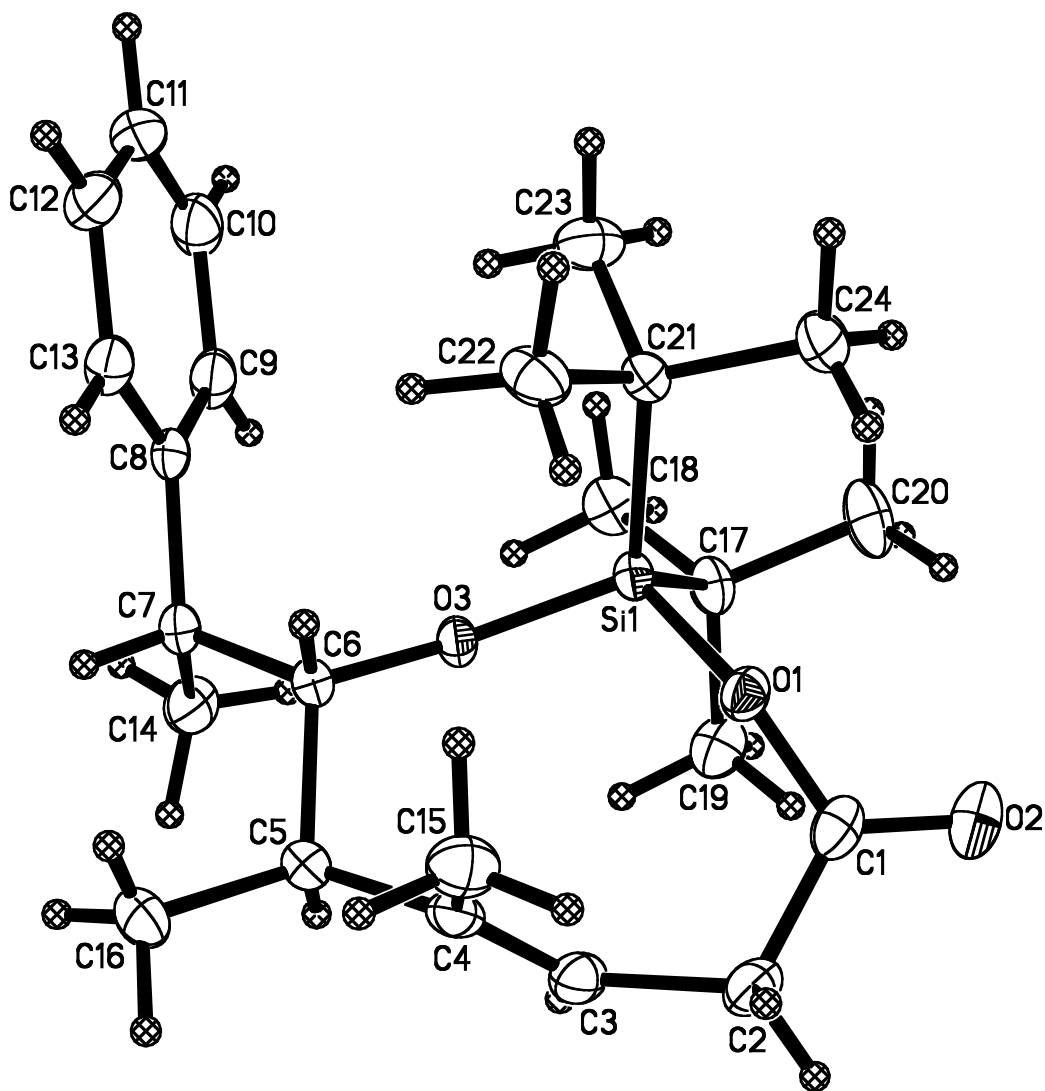
$$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$$

$$R1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$$

Goof = $S = [\Sigma[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

The thermal ellipsoid plot is shown at the 50% probability level.



Table 1. Crystal data and structure refinement for **21**.

Identification code	21 (Christian Ventocilla)
Empirical formula	C ₂₄ H ₃₈ O ₃ Si
Formula weight	402.63
Temperature	103(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$

Unit cell dimensions	a = 9.5046(6) Å	β = 76.7490(10)°.
	b = 10.9462(6) Å	γ = 84.1220(10)°.
	c = 11.6723(7) Å	α = 88.0320(10)°.
Volume	1175.76(12) Å ³	
Z	2	
Density (calculated)	1.137 Mg/m ³	
Absorption coefficient	0.120 mm ⁻¹	
F(000)	440	
Crystal color	colorless	
Crystal size	0.25 x 0.21 x 0.13 mm ³	
Theta range for data collection	1.80 to 27.10°	
Index ranges	-12 ≤ h ≤ 12, -14 ≤ k ≤ 14, -14 ≤ l ≤ 14	
Reflections collected	13579	
Independent reflections	5135 [R(int) = 0.0152]	
Completeness to theta = 25.50°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9845 and 0.9705	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5135 / 0 / 405	
Goodness-of-fit on F ²	1.043	
Final R indices [I > 2σ(I) = 4614 data]	R1 = 0.0340, wR2 = 0.0901	
R indices (all data, 0.78Å)	R1 = 0.0379, wR2 = 0.0931	
Largest diff. peak and hole	0.389 and -0.197 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **21**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	2162(1)	1839(1)	6790(1)	16(1)
O(1)	1069(1)	1192(1)	6070(1)	20(1)
O(2)	1226(1)	919(1)	4227(1)	29(1)
O(3)	1429(1)	3002(1)	7301(1)	17(1)
C(1)	596(1)	1349(1)	4997(1)	23(1)
C(2)	-822(2)	2030(1)	4876(1)	27(1)
C(3)	-953(1)	3028(1)	5574(1)	24(1)
C(4)	-1375(1)	2832(1)	6721(1)	21(1)
C(5)	-1020(1)	3792(1)	7392(1)	21(1)
C(6)	270(1)	3293(1)	8083(1)	17(1)
C(7)	785(1)	4242(1)	8742(1)	19(1)
C(8)	1847(1)	3637(1)	9598(1)	20(1)
C(9)	3282(1)	3925(1)	9426(1)	25(1)
C(10)	4192(1)	3371(1)	10266(1)	33(1)
C(11)	3686(2)	2522(1)	11280(1)	36(1)
C(12)	2268(2)	2213(1)	11463(1)	32(1)
C(13)	1358(1)	2772(1)	10627(1)	24(1)
C(14)	1288(2)	5462(1)	7896(1)	27(1)
C(15)	-2047(1)	1636(1)	7436(1)	28(1)
C(16)	-2266(1)	4115(1)	8222(1)	29(1)
C(17)	3633(1)	2634(1)	5686(1)	22(1)
C(18)	4573(1)	3385(1)	6270(1)	27(1)
C(19)	2986(2)	3570(1)	4672(1)	27(1)
C(20)	4566(2)	1683(1)	5156(1)	33(1)
C(21)	2621(1)	423(1)	7976(1)	19(1)
C(22)	1360(1)	101(1)	8923(1)	28(1)
C(23)	3898(2)	652(1)	8603(1)	30(1)
C(24)	2928(2)	-732(1)	7442(1)	29(1)

Table 3. Bond lengths [Å] and angles [°] for **21**.

Si(1)-O(3)	1.6324(8)
Si(1)-O(1)	1.6696(8)
Si(1)-C(17)	1.8901(12)
Si(1)-C(21)	1.8990(11)
O(1)-C(1)	1.3460(14)
O(2)-C(1)	1.2052(15)
O(3)-C(6)	1.4319(12)
C(1)-C(2)	1.5209(18)
C(2)-C(3)	1.5004(16)
C(2)-H(2A)	1.026(17)
C(2)-H(2B)	1.001(16)
C(3)-C(4)	1.3278(17)
C(3)-H(3A)	0.974(15)
C(4)-C(15)	1.5052(17)
C(4)-C(5)	1.5124(16)
C(5)-C(16)	1.5362(16)
C(5)-C(6)	1.5512(15)
C(5)-H(5A)	0.980(15)
C(6)-C(7)	1.5458(15)
C(6)-H(6A)	0.989(13)
C(7)-C(8)	1.5212(15)
C(7)-C(14)	1.5264(17)
C(7)-H(7A)	0.955(14)
C(8)-C(9)	1.3940(17)
C(8)-C(13)	1.3963(17)
C(9)-C(10)	1.3937(19)
C(9)-H(9A)	0.940(16)
C(10)-C(11)	1.381(2)
C(10)-H(10A)	0.978(19)
C(11)-C(12)	1.384(2)
C(11)-H(11A)	0.950(18)
C(12)-C(13)	1.3921(18)
C(12)-H(12A)	0.958(17)
C(13)-H(13A)	0.965(15)

C(14)-H(14A)	0.964(16)
C(14)-H(14B)	0.977(16)
C(14)-H(14C)	1.001(17)
C(15)-H(15A)	0.96(2)
C(15)-H(15B)	0.98(2)
C(15)-H(15C)	0.96(2)
C(16)-H(16A)	0.964(17)
C(16)-H(16B)	0.968(17)
C(16)-H(16C)	0.967(17)
C(17)-C(20)	1.5398(16)
C(17)-C(18)	1.5403(17)
C(17)-C(19)	1.5424(17)
C(18)-H(18A)	0.961(17)
C(18)-H(18B)	1.010(16)
C(18)-H(18C)	0.961(18)
C(19)-H(19A)	0.962(17)
C(19)-H(19B)	0.970(18)
C(19)-H(19C)	0.992(16)
C(20)-H(20A)	0.982(17)
C(20)-H(20B)	0.993(17)
C(20)-H(20C)	0.973(17)
C(21)-C(23)	1.5346(16)
C(21)-C(22)	1.5367(16)
C(21)-C(24)	1.5400(16)
C(22)-H(22A)	0.975(17)
C(22)-H(22B)	1.035(17)
C(22)-H(22C)	0.985(18)
C(23)-H(23A)	0.985(17)
C(23)-H(23B)	0.971(17)
C(23)-H(23C)	0.952(17)
C(24)-H(21A)	0.987(17)
C(24)-H(21B)	0.961(18)
C(24)-H(21C)	0.99(2)
O(3)-Si(1)-O(1)	112.73(4)
O(3)-Si(1)-C(17)	102.66(5)

O(1)-Si(1)-C(17)	108.33(5)
O(3)-Si(1)-C(21)	114.28(5)
O(1)-Si(1)-C(21)	100.65(5)
C(17)-Si(1)-C(21)	118.43(5)
C(1)-O(1)-Si(1)	140.92(7)
C(6)-O(3)-Si(1)	141.87(7)
O(2)-C(1)-O(1)	121.64(11)
O(2)-C(1)-C(2)	123.70(11)
O(1)-C(1)-C(2)	114.55(10)
C(3)-C(2)-C(1)	110.70(10)
C(3)-C(2)-H(2A)	110.8(9)
C(1)-C(2)-H(2A)	105.4(9)
C(3)-C(2)-H(2B)	113.9(9)
C(1)-C(2)-H(2B)	107.4(9)
H(2A)-C(2)-H(2B)	108.2(13)
C(4)-C(3)-C(2)	124.80(11)
C(4)-C(3)-H(3A)	118.1(8)
C(2)-C(3)-H(3A)	115.8(8)
C(3)-C(4)-C(15)	123.82(11)
C(3)-C(4)-C(5)	118.82(11)
C(15)-C(4)-C(5)	116.98(10)
C(4)-C(5)-C(16)	113.49(10)
C(4)-C(5)-C(6)	108.17(9)
C(16)-C(5)-C(6)	111.12(9)
C(4)-C(5)-H(5A)	107.5(8)
C(16)-C(5)-H(5A)	109.6(8)
C(6)-C(5)-H(5A)	106.7(8)
O(3)-C(6)-C(7)	108.22(9)
O(3)-C(6)-C(5)	110.70(8)
C(7)-C(6)-C(5)	112.55(9)
O(3)-C(6)-H(6A)	108.9(7)
C(7)-C(6)-H(6A)	108.8(7)
C(5)-C(6)-H(6A)	107.6(7)
C(8)-C(7)-C(14)	114.15(10)
C(8)-C(7)-C(6)	111.19(9)
C(14)-C(7)-C(6)	112.16(9)

C(8)-C(7)-H(7A)	106.9(8)
C(14)-C(7)-H(7A)	106.5(8)
C(6)-C(7)-H(7A)	105.2(9)
C(9)-C(8)-C(13)	118.06(11)
C(9)-C(8)-C(7)	123.44(11)
C(13)-C(8)-C(7)	118.48(10)
C(10)-C(9)-C(8)	120.61(12)
C(10)-C(9)-H(9A)	119.8(9)
C(8)-C(9)-H(9A)	119.6(9)
C(11)-C(10)-C(9)	120.46(13)
C(11)-C(10)-H(10A)	119.0(10)
C(9)-C(10)-H(10A)	120.5(10)
C(10)-C(11)-C(12)	119.87(12)
C(10)-C(11)-H(11A)	119.8(11)
C(12)-C(11)-H(11A)	120.3(11)
C(11)-C(12)-C(13)	119.64(13)
C(11)-C(12)-H(12A)	121.1(10)
C(13)-C(12)-H(12A)	119.3(10)
C(12)-C(13)-C(8)	121.36(12)
C(12)-C(13)-H(13A)	120.1(9)
C(8)-C(13)-H(13A)	118.5(9)
C(7)-C(14)-H(14A)	110.8(9)
C(7)-C(14)-H(14B)	112.3(9)
H(14A)-C(14)-H(14B)	106.7(13)
C(7)-C(14)-H(14C)	109.4(10)
H(14A)-C(14)-H(14C)	109.8(13)
H(14B)-C(14)-H(14C)	107.6(13)
C(4)-C(15)-H(15A)	112.5(11)
C(4)-C(15)-H(15B)	109.3(11)
H(15A)-C(15)-H(15B)	109.4(16)
C(4)-C(15)-H(15C)	111.7(11)
H(15A)-C(15)-H(15C)	108.0(16)
H(15B)-C(15)-H(15C)	105.7(15)
C(5)-C(16)-H(16A)	112.2(10)
C(5)-C(16)-H(16B)	111.2(10)
H(16A)-C(16)-H(16B)	107.6(13)

C(5)-C(16)-H(16C)	111.1(10)
H(16A)-C(16)-H(16C)	107.6(13)
H(16B)-C(16)-H(16C)	106.8(14)
C(20)-C(17)-C(18)	108.81(11)
C(20)-C(17)-C(19)	108.64(10)
C(18)-C(17)-C(19)	107.46(10)
C(20)-C(17)-Si(1)	111.93(8)
C(18)-C(17)-Si(1)	110.63(8)
C(19)-C(17)-Si(1)	109.24(8)
C(17)-C(18)-H(18A)	109.1(9)
C(17)-C(18)-H(18B)	111.2(9)
H(18A)-C(18)-H(18B)	107.7(13)
C(17)-C(18)-H(18C)	112.6(10)
H(18A)-C(18)-H(18C)	107.9(14)
H(18B)-C(18)-H(18C)	108.2(13)
C(17)-C(19)-H(19A)	111.9(10)
C(17)-C(19)-H(19B)	108.5(10)
H(19A)-C(19)-H(19B)	105.9(13)
C(17)-C(19)-H(19C)	112.5(9)
H(19A)-C(19)-H(19C)	109.6(13)
H(19B)-C(19)-H(19C)	108.3(13)
C(17)-C(20)-H(20A)	111.9(9)
C(17)-C(20)-H(20B)	109.1(10)
H(20A)-C(20)-H(20B)	106.6(13)
C(17)-C(20)-H(20C)	112.5(10)
H(20A)-C(20)-H(20C)	109.8(13)
H(20B)-C(20)-H(20C)	106.7(13)
C(23)-C(21)-C(22)	107.47(10)
C(23)-C(21)-C(24)	109.09(10)
C(22)-C(21)-C(24)	107.31(10)
C(23)-C(21)-Si(1)	112.56(8)
C(22)-C(21)-Si(1)	109.77(8)
C(24)-C(21)-Si(1)	110.47(8)
C(21)-C(22)-H(22A)	107.1(9)
C(21)-C(22)-H(22B)	112.1(9)
H(22A)-C(22)-H(22B)	109.5(13)

C(21)-C(22)-H(22C)	111.2(10)
H(22A)-C(22)-H(22C)	108.7(14)
H(22B)-C(22)-H(22C)	108.1(13)
C(21)-C(23)-H(23A)	112.5(9)
C(21)-C(23)-H(23B)	109.2(10)
H(23A)-C(23)-H(23B)	107.1(13)
C(21)-C(23)-H(23C)	111.8(10)
H(23A)-C(23)-H(23C)	107.0(14)
H(23B)-C(23)-H(23C)	109.1(14)
C(21)-C(24)-H(21A)	109.4(9)
C(21)-C(24)-H(21B)	112.6(10)
H(21A)-C(24)-H(21B)	107.3(13)
C(21)-C(24)-H(21C)	111.6(11)
H(21A)-C(24)-H(21C)	106.8(14)
H(21B)-C(24)-H(21C)	108.9(14)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **21**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Si(1)	17(1)	15(1)	16(1)	-6(1)	0(1)	1(1)
O(1)	25(1)	18(1)	18(1)	-6(1)	-4(1)	-1(1)
O(2)	41(1)	26(1)	22(1)	-10(1)	3(1)	-9(1)
O(3)	18(1)	18(1)	18(1)	-8(1)	0(1)	1(1)
C(1)	33(1)	16(1)	19(1)	-4(1)	-2(1)	-8(1)
C(2)	40(1)	21(1)	23(1)	-6(1)	-12(1)	1(1)
C(3)	28(1)	19(1)	26(1)	-6(1)	-10(1)	2(1)
C(4)	18(1)	20(1)	27(1)	-6(1)	-8(1)	4(1)
C(5)	20(1)	21(1)	22(1)	-7(1)	-4(1)	4(1)
C(6)	18(1)	18(1)	17(1)	-6(1)	-1(1)	3(1)
C(7)	22(1)	19(1)	18(1)	-8(1)	-2(1)	3(1)
C(8)	23(1)	20(1)	19(1)	-11(1)	-3(1)	4(1)
C(9)	25(1)	30(1)	24(1)	-13(1)	0(1)	0(1)
C(10)	23(1)	47(1)	37(1)	-24(1)	-8(1)	7(1)
C(11)	40(1)	43(1)	30(1)	-17(1)	-17(1)	18(1)
C(12)	47(1)	30(1)	20(1)	-6(1)	-6(1)	8(1)
C(13)	28(1)	25(1)	20(1)	-9(1)	-1(1)	1(1)
C(14)	39(1)	18(1)	27(1)	-6(1)	-7(1)	0(1)
C(15)	25(1)	28(1)	32(1)	-5(1)	-7(1)	-2(1)
C(16)	21(1)	38(1)	32(1)	-16(1)	-3(1)	9(1)
C(17)	22(1)	19(1)	23(1)	-7(1)	4(1)	-1(1)
C(18)	22(1)	25(1)	32(1)	-7(1)	0(1)	-4(1)
C(19)	34(1)	25(1)	21(1)	-2(1)	1(1)	-7(1)
C(20)	33(1)	28(1)	38(1)	-13(1)	15(1)	-1(1)
C(21)	20(1)	17(1)	20(1)	-5(1)	-2(1)	2(1)
C(22)	27(1)	24(1)	26(1)	4(1)	3(1)	4(1)
C(23)	31(1)	26(1)	34(1)	-3(1)	-14(1)	-1(1)
C(24)	42(1)	20(1)	28(1)	-8(1)	-6(1)	8(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **21**.

	x	y	z	U(eq)
H(2A)	-1570(17)	1351(16)	5199(14)	35(4)
H(2B)	-907(17)	2355(15)	4012(14)	34(4)
H(3A)	-513(15)	3827(14)	5186(13)	25(4)
H(5A)	-709(15)	4552(14)	6807(13)	23(3)
H(6A)	-23(13)	2516(12)	8668(11)	13(3)
H(7A)	-34(15)	4452(13)	9207(12)	22(3)
H(9A)	3633(16)	4512(15)	8744(14)	31(4)
H(10A)	5200(20)	3573(16)	10144(15)	45(5)
H(11A)	4314(19)	2155(17)	11850(15)	43(5)
H(12A)	1896(17)	1631(16)	12164(15)	37(4)
H(13A)	367(16)	2567(14)	10752(12)	25(4)
H(14A)	1996(17)	5295(15)	7296(14)	32(4)
H(14B)	1717(16)	6024(15)	8299(14)	31(4)
H(14C)	463(18)	5917(16)	7516(14)	37(4)
H(15A)	-2290(20)	1089(18)	6949(17)	51(5)
H(15B)	-2900(20)	1841(18)	7907(17)	56(5)
H(15C)	-1440(20)	1177(18)	7997(17)	52(5)
H(16A)	-2119(17)	4883(16)	8462(14)	34(4)
H(16B)	-2419(17)	3455(16)	8931(15)	36(4)
H(16C)	-3136(18)	4211(15)	7845(14)	36(4)
H(18A)	5336(17)	3750(15)	5702(14)	34(4)
H(18B)	4023(17)	4093(15)	6536(14)	34(4)
H(18C)	4979(18)	2873(16)	6941(15)	41(4)
H(19A)	2469(17)	3151(15)	4211(14)	34(4)
H(19B)	3751(18)	4002(16)	4132(15)	40(4)
H(19C)	2368(17)	4208(15)	4958(13)	31(4)
H(20A)	4012(17)	1179(16)	4773(14)	35(4)
H(20B)	5269(18)	2145(16)	4533(15)	37(4)
H(20C)	5102(18)	1133(16)	5740(15)	37(4)
H(21A)	3120(17)	-1468(16)	8077(14)	33(4)

H(21B)	3740(19)	-624(16)	6867(15)	39(4)
H(21C)	2100(20)	-944(18)	7072(16)	51(5)
H(22A)	1603(17)	-676(16)	9469(14)	35(4)
H(22B)	1146(17)	800(16)	9383(15)	39(4)
H(22C)	498(19)	-34(16)	8568(15)	40(4)
H(23A)	4780(18)	768(15)	8070(14)	37(4)
H(23B)	4040(17)	-72(16)	9240(15)	38(4)
H(23C)	3766(17)	1380(16)	8920(14)	37(4)

Table 6. Torsion angles [°] for **21**.

O(3)-Si(1)-O(1)-C(1)	83.76(13)
C(17)-Si(1)-O(1)-C(1)	-29.14(13)
C(21)-Si(1)-O(1)-C(1)	-154.07(12)
O(1)-Si(1)-O(3)-C(6)	59.92(12)
C(17)-Si(1)-O(3)-C(6)	176.25(11)
C(21)-Si(1)-O(3)-C(6)	-54.22(12)
Si(1)-O(1)-C(1)-O(2)	86.27(15)
Si(1)-O(1)-C(1)-C(2)	-97.41(14)
O(2)-C(1)-C(2)-C(3)	-148.03(12)
O(1)-C(1)-C(2)-C(3)	35.73(14)
C(1)-C(2)-C(3)-C(4)	-84.13(15)
C(2)-C(3)-C(4)-C(15)	-12.21(19)
C(2)-C(3)-C(4)-C(5)	160.46(11)
C(3)-C(4)-C(5)-C(16)	135.41(12)
C(15)-C(4)-C(5)-C(16)	-51.42(14)
C(3)-C(4)-C(5)-C(6)	-100.80(12)
C(15)-C(4)-C(5)-C(6)	72.37(13)
Si(1)-O(3)-C(6)-C(7)	141.52(10)
Si(1)-O(3)-C(6)-C(5)	-94.69(12)
C(4)-C(5)-C(6)-O(3)	55.16(12)
C(16)-C(5)-C(6)-O(3)	-179.64(10)
C(4)-C(5)-C(6)-C(7)	176.42(9)
C(16)-C(5)-C(6)-C(7)	-58.38(13)
O(3)-C(6)-C(7)-C(8)	-68.56(11)
C(5)-C(6)-C(7)-C(8)	168.78(9)
O(3)-C(6)-C(7)-C(14)	60.62(12)
C(5)-C(6)-C(7)-C(14)	-62.04(13)
C(14)-C(7)-C(8)-C(9)	-18.21(15)
C(6)-C(7)-C(8)-C(9)	109.89(12)
C(14)-C(7)-C(8)-C(13)	160.02(10)
C(6)-C(7)-C(8)-C(13)	-71.87(13)
C(13)-C(8)-C(9)-C(10)	-0.60(17)
C(7)-C(8)-C(9)-C(10)	177.64(11)
C(8)-C(9)-C(10)-C(11)	0.28(19)

C(9)-C(10)-C(11)-C(12)	0.4(2)
C(10)-C(11)-C(12)-C(13)	-0.6(2)
C(11)-C(12)-C(13)-C(8)	0.31(19)
C(9)-C(8)-C(13)-C(12)	0.31(17)
C(7)-C(8)-C(13)-C(12)	-178.02(11)
O(3)-Si(1)-C(17)-C(20)	175.14(9)
O(1)-Si(1)-C(17)-C(20)	-65.41(10)
C(21)-Si(1)-C(17)-C(20)	48.22(11)
O(3)-Si(1)-C(17)-C(18)	53.60(9)
O(1)-Si(1)-C(17)-C(18)	173.05(8)
C(21)-Si(1)-C(17)-C(18)	-73.32(9)
O(3)-Si(1)-C(17)-C(19)	-64.50(9)
O(1)-Si(1)-C(17)-C(19)	54.95(9)
C(21)-Si(1)-C(17)-C(19)	168.58(8)
O(3)-Si(1)-C(21)-C(23)	-72.84(10)
O(1)-Si(1)-C(21)-C(23)	166.08(9)
C(17)-Si(1)-C(21)-C(23)	48.33(10)
O(3)-Si(1)-C(21)-C(22)	46.82(10)
O(1)-Si(1)-C(21)-C(22)	-74.26(9)
C(17)-Si(1)-C(21)-C(22)	167.98(8)
O(3)-Si(1)-C(21)-C(24)	164.95(8)
O(1)-Si(1)-C(21)-C(24)	43.87(9)
C(17)-Si(1)-C(21)-C(24)	-73.88(10)

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