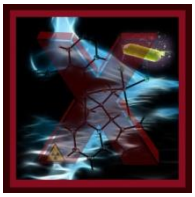

Department of Chemistry

Structure Report 2013
X-RAY
UW-Madison

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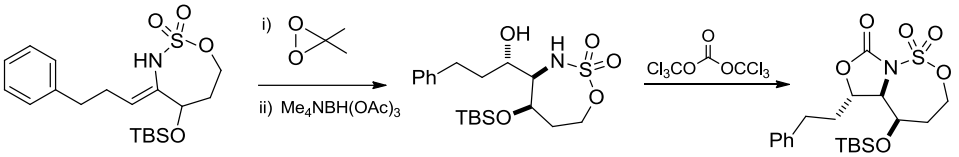
Crystallographic Experimental Section

Crystal Structure of Schomaker32 [CSA5060]



[46] [CSA5060]

Preparation of Crystals: The racemic compound (CSA5060) was dissolved in acetonitrile and crystallized overnight at room temperature by slow vapor diffusion using n-hexanes as solvent. The obtained crystals were air-stable and selected under microscope.

Data Collection: A colorless crystal with approximate dimensions 0.135 x 0.158 x 0.437 mm^3 (block) with a mosaicity of 0.70 was selected under oil under ambient conditions and attached to the tip of a X-ray capillary (MiTeGenMicroMount©). The crystal was mounted in a stream of cold nitrogen at 100.0(15) K and centered in the X-ray beam by using a video camera. The crystal evaluation and data collection were performed on a three-circle Bruker Quazar SMART APEXII diffractometer with Molybdenum K_α(λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 4.96 cm. The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 12 frames collected at intervals of 0.5° in 6° range about ω with the exposure time of 10 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEXII program suite. The final cell constants were calculated from a set of 9893 strong from the actual data collection. The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.70 Å. A total of 35770 reflection data were harvested by collecting 6 sets of frames with 0.6° scans in ω and φ with exposure times of 25 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1,2]

Structure Solution and Refinement: The systematic absences in the diffraction data were consistent for the monoclinic space groups $P2_1/n$. The *E*-statistics strongly suggested the centrosymmetric space group that yielded chemically reasonable and computationally stable results of refinement. [3,4] The systematic absences in the diffraction data were uniquely consistent for the space group $P2_1/n$. A successful solution by the direct methods by using SHELX-2013 provided most non-hydrogen atoms from the *E*-map. Using Olex2, all non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. All atoms of the phenyl group C8-C13 including C6 and C7 are disordered over two positions each. The disorder of the phenyl part was refined with restraints and constraints to give a reasonably stable model.

Table 1. Crystal data collection and structure solution refinement for Schomaker32 [CSA5060]

Parameter	CSA5060	Parameter	CSA5060
empiric formula	$C_{20}H_{31}NO_6SSi$	$\rho_{calc.}$ [g · cm^{-1}]	1.27
MW [g · mol^{-1}]	441.61	crystal size [mm]	0.158 x 0.437 x 0.437
X-ray lab code	Schomaker32	T [K]	100.0(15)
a [Å]	6.9812(5)	radiation type / λ [nm]	Mo K_α / 0.71072
b [Å]	22.2092(24)	μ [mm^{-1}]	0.227
c [Å]	14.9476(8)	F(000)	945.3
α [°]	90.000(0)°	Reflections collected	35165
β [°]	96.282(4)°	Independent reflections	4513 [R_{int} = 0.021, R_{sigma} = 0.0108]
γ [°]	90.000(8)°	Data/restraints/parameters	4513/84/330
V [Å^3]	2303.66(11)	GooF on F^2	1.049
Z	4	Largest diff. peak/hole [eÅ^{-3}]	0.36 / -0.32
crystal system	monoclinic		
crystal color	colorless	Final R_1[a]/ wR_2[b] all data	0.0298/ 0.0739
space group	$P2_1/n$	Final R_1[a]/ wR_2[b] I>2s(I)	0.0287/ 0.0731

[a] $R_1 = \sum| F_o| - | F_c| / | F_o|$;[b] $wR_2 = [\sum\{w(F_o^2 - F_o^2)^2\}/ \sum\{w(F_o^2)^2\}]^{1/2}$

The final least-squares refinement of 330 parameters against 4513 data resulted in R = 0.0287 (based on F^2 for I>2s) and wR2 = 0.0739 (based on F^2 for all data), respectively. The final structure was visualized using Interactive Molecular Graphics. [5]

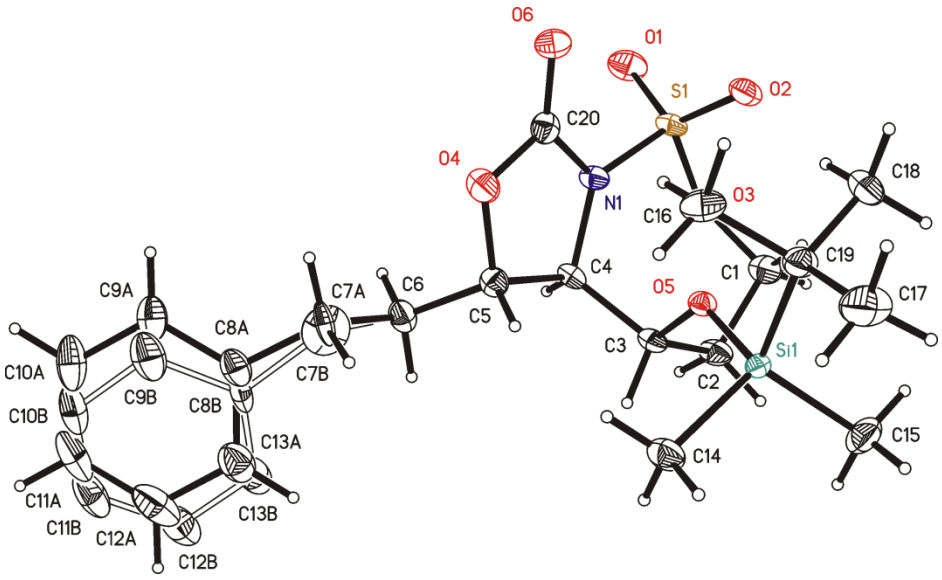


Figure 1. Thermal-ellipsoid of Schomaker32 [CSA5060] are set with 50 % probability. The hydrogen atoms in the disordered phenyl ring were omitted for clarity.

Table 2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Schomaker32 [CSA5060]. U_{eq} is defined as 1/3 of of the trace of the orthogonalized U_{IJ} tensor.

Atom	***x***	***y***	***Z***	**U(eq)**
S1	5027.9(4)	7961.36(14)	7966.90(19)	17.27(8)
Si1	677.4(4)	6468.01(14)	9301.3(2)	13.72(9)
O1	6214.1(13)	8462.5(4)	7817.7(7)	28.1(2)
O2	5865.4(12)	7378.1(4)	8055.8(6)	23.2(2)
O3	3313.7(12)	7976.9(4)	7219.2(6)	22.5(2)
O4	3652.1(13)	8239.7(4)	10308.8(6)	23.9(2)
O5	1604.3(11)	7095.6(4)	8923.3(5)	15.03(17)
O6	6584.5(13)	8072.9(4)	9871.6(6)	24.7(2)
N1	3849.0(14)	8101.8(5)	8854.2(6)	16.1(2)
C1	2042.6(18)	7440.7(6)	7073.8(8)	23.6(3)
C2	237.6(17)	7548.9(6)	7517.9(8)	21.0(3)
C3	591.7(16)	7603.2(5)	8540.9(7)	15.6(2)
C4	1748.9(16)	8161.3(5)	8870.7(8)	15.3(2)
C5	1661.4(17)	8263.9(5)	9890.2(8)	17.6(2)
C6	741.1(18)	8851.9(5)	10123.1(8)	20.6(3)
C14	-997.1(18)	6664.2(6)	10138.6(9)	23.8(3)
C15	-631(2)	6033.5(6)	8360.0(9)	28.6(3)
C16	3835.2(18)	6446.7(6)	10614.0(9)	25.8(3)
C17	2340(2)	5452.3(7)	10209.7(13)	38.4(4)
C18	4296.7(19)	5975.2(6)	9123.6(10)	30.1(3)
C19	2880.2(17)	6065.0(5)	9832.7(9)	20.8(3)
C20	4868.6(18)	8129.4(5)	9696.3(8)	18.9(2)
C7A	684(11)	8891(3)	11168(5)	22.5(10)
C8A	-420(8)	9424(3)	11444(4)	23(1)
C9A	449(8)	9885.7(16)	11956(2)	26.1(8)
C10A	-636(11)	10350.3(14)	12266(2)	34.5(11)
C11A	-2618(11)	10357.1(17)	12057(3)	37.3(13)
C12A	-3505(7)	9905.5(18)	11535(4)	42(1)
C13A	-2417(7)	9433.9(18)	11235(4)	32.5(9)
C7B	510(30)	8945(9)	11047(13)	41(4)
C8B	-950(20)	9433(5)	11311(9)	25(2)
C9B	-320(20)	9859(4)	11976(6)	34.1(19)
C10B	-1600(20)	10307(3)	12215(5)	32(2)
C11B	-3450(20)	10324(4)	11811(8)	38(2)
C12B	-4026(16)	9923(4)	11143(10)	43(2)
C13B	-2775(15)	9480(4)	10895(9)	35(2)

Table 3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for csa5060.
The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+...]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S1	11.66(14)	24.32(16)	16.50(15)	1.91(10)	4.57(11)	2.73(11)
Si1	11.27(15)	15.92(16)	14.00(16)	-1.44(11)	1.55(11)	-3.26(11)
O1	22.1(5)	33.4(5)	30.8(5)	-3.1(4)	11.3(4)	6.9(4)
O2	15.4(4)	28.2(5)	26.2(5)	5.0(3)	2.4(3)	-2.3(4)
O3	17.7(4)	36.0(5)	14.3(4)	3.8(4)	3.7(3)	5.3(3)
O4	22.6(5)	33.1(5)	15.5(4)	6.7(4)	-0.8(3)	-2.4(4)
O5	11.9(4)	16.7(4)	16.2(4)	1.7(3)	0.3(3)	0.1(3)
O6	18.2(4)	29.1(5)	25.3(5)	2.4(4)	-4.1(4)	-0.3(4)
N1	12.4(5)	21.3(5)	14.7(5)	0.4(4)	2.2(4)	1.6(4)
C1	18.3(6)	38.0(7)	14.3(6)	1.4(5)	0.7(5)	-4.0(5)
C2	14.3(6)	33.1(7)	14.9(6)	3.2(5)	-1.0(4)	0.2(5)
C3	11.4(5)	21.1(6)	14.5(5)	3.8(4)	1.8(4)	1.6(4)
C4	13.1(5)	18.3(6)	15.1(5)	4.2(4)	4.2(4)	2.5(4)
C5	18.5(6)	19.0(6)	15.2(5)	0.4(5)	2.6(4)	0.4(4)
C6	23.8(6)	18.4(6)	20.7(6)	0.7(5)	7.8(5)	-1.0(5)
C14	19.8(6)	30.2(7)	22.7(6)	0.7(5)	8.1(5)	0.1(5)
C15	28.2(7)	31.7(7)	25.3(7)	-10.3(6)	0.9(5)	-9.0(5)
C16	17.7(6)	33.9(7)	24.5(7)	-1.3(5)	-3.5(5)	5.3(5)
C17	27.3(7)	22.3(7)	65.6(11)	-0.6(6)	4.3(7)	14.9(7)
C18	21.0(6)	26.1(7)	44.5(8)	5.5(5)	8.9(6)	-4.7(6)
C19	16.2(6)	16.2(6)	30.0(7)	-0.0(4)	3.0(5)	2.6(5)
C20	21.5(6)	16.3(6)	18.5(6)	1.2(5)	0.2(5)	0.5(4)
C7A	41(2)	18.4(19)	9.9(14)	8.2(13)	11.7(14)	-2.0(15)
C8A	30(2)	22.2(15)	19.0(14)	2.6(14)	10.6(13)	2.4(10)
C9A	43(2)	21.4(12)	14.9(11)	3.0(13)	5.6(13)	2.2(8)
C10A	66(3)	17.8(12)	20.5(12)	6.4(14)	9.7(14)	1.3(8)
C11A	56(4)	23.9(14)	38(2)	13(2)	30(2)	5.2(13)
C12A	39.8(19)	35.7(18)	56(2)	9.5(13)	28.6(17)	11.2(16)
C13A	36(2)	25.0(13)	39(2)	-0.1(11)	16.3(16)	0.3(14)
C7B	54(6)	29(4)	40(7)	-5(4)	6(4)	14(3)
C8B	37(5)	13(3)	29(4)	-2(3)	21(3)	-6(2)
C9B	50(5)	31(3)	24(3)	3(3)	16(3)	2.9(19)
C10B	54(6)	21(3)	25(3)	2(3)	20(4)	-2.8(18)
C11B	53(5)	18(3)	50(4)	4(3)	33(3)	2(2)
C12B	43(4)	25(3)	67(5)	-1(2)	31(3)	-4(3)
C13B	36(4)	20(3)	53(5)	-4(2)	24(3)	-5(3)

Table 4. Bond Lengths for Schomaker32 [CSA5060].

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O1	1.4194(10)	C6	C7A	1.569(7)
S1	O2	1.4215(9)	C6	C7B	1.423(18)
S1	O3	1.5459(9)	C16	C19	1.5351(18)
S1	N1	1.6651(10)	C17	C19	1.5357(18)
Si1	O5	1.6616(9)	C18	C19	1.5396(18)
Si1	C14	1.8556(13)	C7A	C8A	1.495(8)
Si1	C15	1.8613(13)	C8A	C9A	1.380(6)
Si1	C19	1.8786(13)	C8A	C13A	1.395(5)
O3	C1	1.4868(16)	C9A	C10A	1.389(4)
O4	C5	1.4613(14)	C10A	C11A	1.385(5)
O4	C20	1.3378(15)	C11A	C12A	1.376(6)
O5	C3	1.4172(14)	C12A	C13A	1.396(5)
O6	C20	1.2044(15)	C7B	C8B	1.57(2)
N1	C4	1.4750(14)	C8B	C9B	1.408(13)
N1	C20	1.3779(15)	C8B	C13B	1.358(12)
C1	C2	1.5064(17)	C9B	C10B	1.408(11)
C2	C3	1.5269(16)	C10B	C11B	1.366(11)
C3	C4	1.5313(16)	C11B	C12B	1.367(11)
C4	C5	1.5485(16)	C12B	C13B	1.391(11)
C5	C6	1.5127(16)			

Table 5. Bond Angles for Schomaker32 [CSA5060].

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	S1	O1	119.23(6)	C6	C5	O4	109.95(10)
O3	S1	O1	106.72(5)	C6	C5	C4	114.65(10)
O3	S1	O2	111.46(5)	C16	C19	Si1	109.02(8)
N1	S1	O1	109.03(6)	C17	C19	Si1	110.79(9)
N1	S1	O2	109.29(5)	C17	C19	C16	108.28(12)
N1	S1	O3	99.25(5)	C18	C19	Si1	109.17(9)
C14	Si1	O5	109.26(5)	C18	C19	C16	109.70(10)
C15	Si1	O5	110.80(5)	C18	C19	C17	109.86(11)
C15	Si1	C14	109.77(6)	O6	C20	O4	124.12(11)
C19	Si1	O5	102.25(5)	N1	C20	O4	109.28(10)
C19	Si1	C14	111.94(6)	N1	C20	O6	126.60(12)
C19	Si1	C15	112.58(6)	C9A	C8A	C7A	122.2(4)
C1	O3	S1	119.36(8)	C13A	C8A	C7A	118.9(5)
C20	O4	C5	111.03(9)	C13A	C8A	C9A	118.7(4)
C3	O5	Si1	127.50(7)	C10A	C9A	C8A	120.9(3)
C4	N1	S1	127.52(8)	C11A	C10A	C9A	120.1(3)
C20	N1	S1	119.01(8)	C12A	C11A	C10A	119.7(3)
C20	N1	C4	113.32(9)	C13A	C12A	C11A	120.2(4)
C2	C1	O3	108.81(10)	C12A	C13A	C8A	120.4(4)
C3	C2	C1	113.72(10)	C9B	C8B	C7B	118.7(10)
C2	C3	O5	111.11(9)	C13B	C8B	C7B	122.7(10)

C4	C3	O5	106.96(9)	C13B	C8B	C9B	118.5(9)
C4	C3	C2	114.09(10)	C10B	C9B	C8B	119.7(8)
C3	C4	N1	114.36(9)	C11B	C10B	C9B	120.1(7)
C5	C4	N1	100.13(9)	C12B	C11B	C10B	119.6(7)
C5	C4	C3	111.09(9)	C13B	C12B	C11B	120.8(8)
C4	C5	O4	106.13(9)	C12B	C13B	C8B	121.1(8)

Table 6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Schomaker32

Atom	***x***	***y***	***z***	**U(eq)**
H1a	1708.4(18)	7371.6(6)	6421.1(8)	28.4(3)
H1b	2718.5(18)	7079.2(6)	7335.5(8)	28.4(3)
H2a	-381.8(17)	7923.5(6)	7271.5(8)	25.2(3)
H2b	-671.0(17)	7213.0(6)	7363.3(8)	25.2(3)
H3	-687.3(16)	7621.2(5)	8782.6(7)	18.7(3)
H4	1259.8(16)	8524.3(5)	8521.7(8)	18.4(3)
H5	926.3(17)	7924.9(5)	10130.6(8)	21.1(3)
H6aa	1491.7(18)	9193.8(5)	9917.9(8)	24.7(3)
H6ab	-584.6(18)	8876.2(5)	9813.2(8)	24.7(3)
H6bc	1531.5(18)	9185.7(5)	9922.6(8)	24.7(3)
H6bd	-543.6(18)	8878.2(5)	9772.1(8)	24.7(3)
H14a	-2066(8)	6904(4)	9847.1(17)	35.7(4)
H14b	-1503(11)	6294.4(6)	10382(5)	35.7(4)
H14c	-306(4)	6898(4)	10629(3)	35.7(4)
H15a	-1024(14)	5643(2)	8584.0(18)	42.8(4)
H15b	-1776(9)	6259(2)	8113(5)	42.8(4)
H15c	217(5)	5970(4)	7888(3)	42.8(4)
H16a	2948(6)	6490(4)	11075(3)	38.7(4)
H16b	5020(8)	6248(2)	10876(4)	38.7(4)
H16c	4147(13)	6845.6(17)	10389.9(16)	38.7(4)
H17a	3496(4)	5260(3)	10515(7)	57.7(6)
H17b	1393(14)	5510.9(8)	10639(6)	57.7(6)
H17c	1788(16)	5194(2)	9715.4(16)	57.7(6)
H18a	4641(12)	6367.7(7)	8888(5)	45.2(5)
H18b	5462(7)	5774(4)	9402(2)	45.2(5)
H18c	3689(6)	5727(4)	8630(4)	45.2(5)
H7Aa	88(11)	8519(3)	11377(5)	27.0(12)
H7Ab	2019(11)	8912(3)	11467(5)	27.0(12)
H9A	1809(8)	9886.2(16)	12098(2)	31.4(10)
H10A	-18(11)	10663.6(14)	12621(2)	41.4(13)
H11A	-3363(11)	10672.5(17)	12274(3)	44.7(15)
H12A	-4860(7)	9914.5(18)	11378(4)	50.4(12)
H13A	-3040(7)	9118.1(18)	10887(4)	39(1)
H7Ba	120(30)	8555(9)	11294(13)	49(4)
H7Bb	1790(30)	9047(9)	11361(13)	49(4)
H9B	960(20)	9844(4)	12263(6)	41(2)
H10B	-1170(20)	10598(3)	12659(5)	39(3)

H11B	-4330(20)	10614(4)	11993(8)	46(3)
H12B	-5296(16)	9946(4)	10844(10)	51(3)
H13B	-3204(15)	9207(4)	10427(9)	42(2)

Table 7. Atomic Occupancy for Schomaker32 [CSA5060].

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
H6aa	0.674(14)	H6ab	0.674(14)	H6bc	0.326(14)
H6bd	0.326(14)	C7A	0.674(14)	H7Aa	0.674(14)
H7Ab	0.674(14)	C8A	0.674(14)	C9A	0.674(14)
H9A	0.674(14)	C10A	0.674(14)	H10A	0.674(14)
C11A	0.674(14)	H11A	0.674(14)	C12A	0.674(14)
H12A	0.674(14)	C13A	0.674(14)	H13A	0.674(14)
C7B	0.326(14)	H7Ba	0.326(14)	H7Bb	0.326(14)
C8B	0.326(14)	C9B	0.326(14)	H9B	0.326(14)
C10B	0.326(14)	H10B	0.326(14)	C11B	0.326(14)
H11B	0.326(14)	C12B	0.326(14)	H12B	0.326(14)
C13B	0.326(14)	H13B	0.326(14)		

References:

[1] BRUKER-AXS. (2007-2013), APEX2 (Ver. 2013.2-0), SADABS (2012-1)

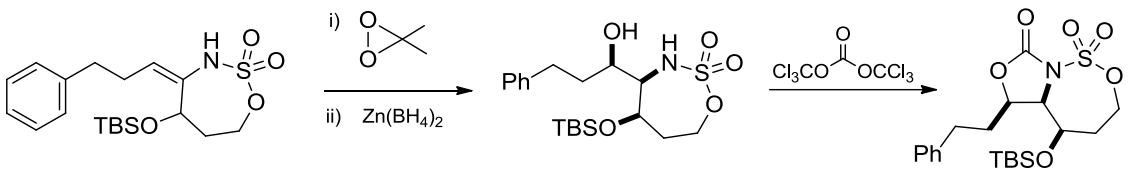
[2] SAINT+ (Ver. 8.30C) Software Reference Manuals, BRUKER-AXS, Madison, Wisconsin, USA.

[3] G. M. Sheldrick, *Acta Cryst.*, **2008**, *A64*, 112-122.

[4] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. L. Howard, H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339-341.

[5] XP – X-Ray Crystal Structure Visualization BRUKER, AXS, **1998**, V5.1

Crystal Structure of Schomaker31 [CSA5062]



[26] [CSA5062]

Preparation of Crystals: The racemic compound (CSA5062) was dissolved in acetonitrile and crystallized by slow evaporation at 7 °C. The obtained air-stable crystals were selected under microscope.

Data Collection: A colorless crystal with approximate dimensions 0.032 x 0.125 x 0.403 mm^3 (block) with a mosaicity of 0.68 was selected under oil under ambient conditions and attached to the tip of a X-ray capillary (MiTeGenMicroMount©). The crystal was mounted in a stream of cold nitrogen at 100.0(15) K and centered in the X-ray beam by using a video camera. The crystal evaluation and data collection were performed on a three-circle Bruker Quazar SMART APEXII ("GROMIT") diffractometer with Molybdenum K_a(λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 4.96 cm. The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 12 frames collected at intervals of 0.5° in 6° range about ω with the exposure time of 10 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEXII program suite. The final cell constants were calculated from a set of 9196 strong from the actual data collection. The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.70 Å. A total of 27764 reflection data were harvested by collecting 6 sets of frames with 0.6° scans in ω and φ with exposure times of 20 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [6,7]

Structure Solution and Refinement: The systematic absences in the diffraction data were consistent for the triclinic space groups P1 and $P\bar{1}$. The R_{int}-value was 0.043 and suggested a successful structure refinement. The *E*-statistics strongly suggested the centrosymmetric space group that yielded chemically reasonable and computationally stable results of refinement. [8] A successful solution by the "direct methods" by using SHELX-2013 [9] provided most non-hydrogen atoms from the *E*-map. Using Olex2, [10] all non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

Table 8. Crystal data collection and structure solution refinement for Schomaker31 [CSA5062]

Parameter	CSA5062	Parameter	CSA5062
empiric formula	$C_{20}H_{31}NO_6SSi$	$\rho_{calc.}$ [g · cm^{-1}]	1.46
MW [g · mol^{-1}]	441.61	crystal size [mm]	0.032 x 0.125 x 0.403
X-ray lab code	Schomaker31	T [K]	100.0(15)
a [Å]	7.2477(28)	radiation type / λ [nm]	Mo K_α / 0.71072
b [Å]	12.2307(40)	μ [mm^{-1}]	0.230
c [Å]	12.4387(41)	F(000)	911.8
α [°]	87.0850(13)	Reflections collected	27763
β [°]	81.980(7)	Independent reflections	5586 [R_{int} = 0.041]
γ [°]	89.975(11)	Data/restraints/parameters	5586/0/262
V [Å^3]	1091.06(14)	GooF on F^2	1.047
Z	2	Largest diff. peak/hole [eÅ^{-3}]	0.76 / -0.22
crystal system	triclinic		
crystal color	colorless	Final R_1[a]/ wR_2[b] all data	0.0424/ 0.0879
space group	$P\bar{1}$	Final R_1[a]/ wR_2[b] I>2s(I)	0.0341/ 0.0830

[a] $R_1 = \sum \left| F_o \right| - \left| F_c \right| / \left| F_o \right|$;[b] $wR_2 = [\sum\{w(F_o^2 - F_o^2)^2\} / \sum\{w(F_o^2)^2\}]^{1/2}$

The final least-squares refinement of 262 parameters against 5586 data resulted in R = 0.0341 (based on F^2 for I>2s) and wR2 = 0.0879 (based on F^2 for all data), respectively. The final structure was visualized using Interactive Molecular Graphics. [5]

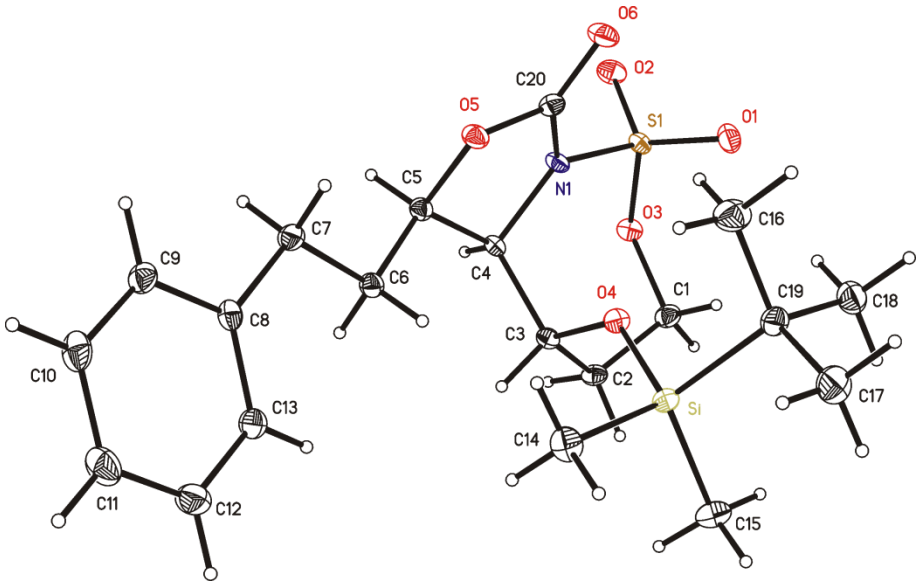


Figure 2. Thermal-ellipsoid of Schomaker31 [CSA5062] are set with 50 % probability

Table 9. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Schomaker31 [CSA5062]. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	7915.6(4)	9368.8(3)	1494.0(3)	10.60(8)
Si	11637.2(5)	7514.7(3)	4206.1(3)	10.91(9)
O4	10953.6(13)	7902.7(8)	3028.7(8)	11.56(19)
O6	6323.1(13)	7137.6(8)	2019.4(9)	15.8(2)
O2	6924.9(14)	9582.3(9)	600.6(9)	16.2(2)
O5	9088.0(13)	6349.5(8)	1498.5(8)	12.9(2)
N1	8952.9(15)	8160.5(9)	1346.1(9)	10.3(2)
O3	9651.2(13)	10130.6(8)	1306.5(8)	12.4(2)
O1	6968.2(14)	9432.3(8)	2569.7(8)	15.9(2)
C6	12406.6(18)	6000.0(11)	1188.9(11)	11.9(3)
C2	12472.7(18)	9480.7(11)	2010.1(11)	11.6(3)
C20	7948.5(18)	7210.0(11)	1667.9(11)	11.4(3)
C7	12127.6(19)	4807.9(11)	914.9(12)	13.5(3)
C14	12909(2)	6193.3(12)	4102.9(12)	17.3(3)
C4	10974.2(17)	7951.4(11)	1104.5(11)	9.7(2)
C3	12037.3(18)	8255.0(11)	2038.0(11)	10.0(2)
C8	13638.1(19)	4034.8(11)	1193.5(11)	12.1(3)
C10	14877(2)	2189.2(12)	1189.1(13)	17.5(3)
C19	9360(2)	7380.2(12)	5140.9(11)	14.2(3)
C5	10864.4(18)	6721.0(11)	881.7(11)	10.9(3)
C13	15122(2)	4366.7(12)	1703.9(12)	15.1(3)
C1	10797.9(19)	10211.6(11)	2202.3(12)	13.7(3)
C9	13542(2)	2931.6(11)	938.4(12)	14.3(3)
C11	16334(2)	2529.4(13)	1713.3(13)	20.6(3)
C18	8429(2)	8503.7(13)	5270.1(13)	19.0(3)
C17	9715(2)	6926.1(14)	6264.0(12)	21.0(3)
C15	13223(2)	8539.2(13)	4669.3(13)	19.0(3)
C16	8035(2)	6604.7(13)	4677.1(13)	20.6(3)
C12	16452(2)	3620.9(13)	1965.7(13)	19.9(3)

Table 10. Anisotropic Displacement Parameters (Å^2×10^3) for Schomaker31 [CSA5062].
The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka\times b\times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	8.49(15)	10.62(15)	12.50(16)	0.18(12)	-0.92(11)	1.67(11)
Si	11.65(17)	10.54(18)	10.84(18)	0.41(14)	-2.86(13)	-0.93(13)
O4	11.7(4)	12.5(5)	10.3(5)	1.7(4)	-1.3(3)	-2.1(3)
O6	9.2(4)	16.5(5)	21.5(5)	-0.2(4)	-1.5(4)	-1.8(4)
O2	13.4(5)	17.7(5)	18.1(5)	2.3(4)	-5.8(4)	2.7(4)
O5	9.5(4)	10.5(5)	18.5(5)	-1.5(4)	-0.9(4)	-1.1(3)
N1	6.6(5)	9.3(5)	15.1(6)	-0.2(4)	-1.5(4)	1.1(4)
O3	11.8(4)	11.0(5)	14.3(5)	1.9(4)	-2.4(4)	-0.8(3)
O1	14.5(5)	16.4(5)	15.7(5)	-2.6(4)	2.5(4)	0.8(4)
C6	11.0(6)	10.0(6)	14.8(7)	-1.6(5)	-2.3(5)	1.2(5)
C2	11.0(6)	9.8(6)	14.4(7)	0.6(5)	-3.4(5)	-2.5(5)

C20	11.7(6)	11.3(6)	11.8(6)	-0.3(5)	-4.3(5)	-0.2(5)
C7	13.2(6)	10.4(6)	17.5(7)	-2.9(5)	-3.8(5)	0.2(5)
C14	19.5(7)	15.5(7)	16.4(7)	2.5(6)	-1.9(5)	2.5(5)
C4	7.2(6)	10.5(6)	11.0(6)	-0.4(5)	-0.5(4)	1.3(4)
C3	8.3(6)	10.3(6)	11.1(6)	0.8(5)	-1.0(5)	-0.6(4)
C8	13.0(6)	10.8(6)	11.8(6)	-0.4(5)	1.3(5)	0.6(5)
C10	20.9(7)	9.0(6)	21.5(8)	-1.3(5)	1.1(6)	0.4(5)
C19	14.8(6)	17.0(7)	10.5(6)	0.6(5)	-1.7(5)	-0.6(5)
C5	9.5(6)	10.5(6)	12.5(6)	-1.1(5)	-0.5(5)	-0.6(5)
C13	15.3(6)	11.6(6)	19.0(7)	-3.2(5)	-3.4(5)	1.4(5)
C1	14.5(6)	11.1(6)	16.1(7)	-1.8(5)	-4.7(5)	-0.8(5)
C9	15.0(6)	11.4(6)	16.3(7)	-2.2(5)	-0.8(5)	-2.4(5)
C11	19.6(7)	15.6(7)	26.7(8)	0.4(6)	-3.7(6)	5.9(6)
C18	17.6(7)	21.3(7)	17.8(7)	-1.8(6)	-1.6(5)	3.7(6)
C17	22.4(8)	26.8(8)	13.3(7)	3.5(6)	-1.8(6)	2.1(6)
C15	18.3(7)	19.5(7)	20.5(8)	-0.7(6)	-8.0(6)	-3.8(6)
C16	18.3(7)	23.4(8)	19.7(8)	1.7(6)	-1.9(6)	-7.0(6)
C12	17.0(7)	18.1(7)	26.2(8)	-3.0(6)	-7.7(6)	2.8(6)

Table 11. Bond Lengths for Schomaker31 CSA5062].

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
S1	O2	1.4210(11)	C6	C5	1.5053(19)
S1	N1	1.6626(12)	C2	C3	1.5303(19)
S1	O3	1.5517(11)	C2	C1	1.5046(19)
S1	O1	1.4210(11)	C7	C8	1.5143(19)
Si	O4	1.6630(11)	C4	C3	1.5369(19)
Si	C14	1.8599(16)	C4	C5	1.5445(19)
Si	C19	1.8853(16)	C8	C13	1.391(2)
Si	C15	1.8610(16)	C8	C9	1.4016(19)
O4	C3	1.4183(16)	C10	C9	1.386(2)
O6	C20	1.2001(17)	C10	C11	1.388(2)
O5	C20	1.3421(16)	C19	C18	1.534(2)
O5	C5	1.4668(16)	C19	C17	1.539(2)
N1	C20	1.3878(18)	C19	C16	1.533(2)
N1	C4	1.4780(17)	C13	C12	1.390(2)
O3	C1	1.4861(17)	C11	C12	1.388(2)
C6	C7	1.5296(19)			

Table 12. Bond Angles for Schomaker31 [CSA5062].

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O2	S1	N1	108.74(6)	N1	C4	C3	112.65(11)
O2	S1	O3	106.16(6)	N1	C4	C5	97.98(10)
O3	S1	N1	99.80(6)	C3	C4	C5	116.37(11)
O1	S1	O2	119.40(7)	O4	C3	C2	111.89(11)
O1	S1	N1	109.62(6)	O4	C3	C4	107.88(10)

O1	S1	O3	111.28(6)	C2	C3	C4	111.77(11)
O4	Si	C14	111.39(6)	C13	C8	C7	122.93(12)
O4	Si	C19	102.46(6)	C13	C8	C9	118.01(13)
O4	Si	C15	111.85(6)	C9	C8	C7	119.06(13)
C14	Si	C19	111.67(7)	C9	C10	C11	120.07(14)
C14	Si	C15	107.27(8)	C18	C19	Si	109.93(10)
C15	Si	C19	112.27(7)	C18	C19	C17	109.01(12)
C3	O4	Si	129.47(9)	C17	C19	Si	109.70(10)
C20	O5	C5	109.18(10)	C16	C19	Si	110.45(10)
C20	N1	S1	119.71(9)	C16	C19	C18	108.63(13)
C20	N1	C4	112.01(11)	C16	C19	C17	109.10(13)
C4	N1	S1	127.12(9)	O5	C5	C6	109.20(11)
C1	O3	S1	118.07(9)	O5	C5	C4	104.76(10)
C5	C6	C7	111.81(11)	C6	C5	C4	117.45(11)
C1	C2	C3	115.10(11)	C12	C13	C8	120.82(13)
O6	C20	O5	124.10(13)	O3	C1	C2	110.32(11)
O6	C20	N1	127.14(13)	C10	C9	C8	121.25(14)
O5	C20	N1	108.75(11)	C10	C11	C12	119.31(14)
C8	C7	C6	114.75(12)	C11	C12	C13	120.53(14)

Table 13. Torsion Angles for Schomaker31 [CSA5062].

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	N1	C20	O6	3.3(2)	C7	C6	C5	C4	-179.53(11)
S1	N1	C20	O5	-178.25(9)	C7	C8	C13	C12	178.51(14)
S1	N1	C4	C3	66.76(15)	C7	C8	C9	C10	-179.17(13)
S1	N1	C4	C5	-170.25(10)	C14	Si	O4	C3	-68.43(12)
S1	O3	C1	C2	98.53(12)	C14	Si	C19	C18	175.74(10)
Si	O4	C3	C2	-85.52(13)	C14	Si	C19	C17	55.88(12)
Si	O4	C3	C4	151.15(9)	C14	Si	C19	C16	-64.41(12)
O4	Si	C19	C18	-64.94(11)	C4	N1	C20	O6	171.82(14)
O4	Si	C19	C17	175.21(10)	C4	N1	C20	O5	-9.71(15)
O4	Si	C19	C16	54.92(11)	C3	C2	C1	O3	-65.04(15)
O2	S1	N1	C20	-82.42(12)	C3	C4	C5	O5	94.42(13)
O2	S1	N1	C4	110.93(12)	C3	C4	C5	C6	-26.92(16)
O2	S1	O3	C1	170.64(9)	C8	C13	C12	C11	0.6(2)
N1	S1	O3	C1	-76.43(10)	C10	C11	C12	C13	0.4(2)
N1	C4	C3	O4	41.40(14)	C19	Si	O4	C3	172.05(11)
N1	C4	C3	C2	-82.01(13)	C5	O5	C20	O6	169.53(13)
N1	C4	C5	O5	-25.82(12)	C5	O5	C20	N1	-9.00(14)
N1	C4	C5	C6	-147.15(12)	C5	C6	C7	C8	179.51(11)
O3	S1	N1	C20	166.67(11)	C5	C4	C3	O4	-70.60(13)
O3	S1	N1	C4	0.02(12)	C5	C4	C3	C2	165.98(11)
O1	S1	N1	C20	49.75(12)	C13	C8	C9	C10	0.3(2)
O1	S1	N1	C4	-116.89(12)	C1	C2	C3	O4	-55.99(15)
O1	S1	O3	C1	39.23(11)	C1	C2	C3	C4	65.12(15)
C6	C7	C8	C13	2.8(2)	C9	C8	C13	C12	-0.9(2)
C6	C7	C8	C9	-177.78(12)	C9	C10	C11	C12	-1.0(2)

C20	O5	C5	C6	149.62(11)	C11	C10	C9	C8	0.7(2)
C20	O5	C5	C4	23.00(14)	C15	Si	O4	C3	51.60(13)
C20	N1	C4	C3	-100.75(13)	C15	Si	C19	C18	55.22(12)
C20	N1	C4	C5	22.24(14)	C15	Si	C19	C17	-64.64(12)
C7	C6	C5	O5	61.46(14)	C15	Si	C19	C16	175.08(10)

Table 14. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for Schomaker31

Atom	***x***	***y***	***z***	**U(eq)**
H6A	12453	6041	1962	14
H6B	13589	6265	806	14
H2A	13270	9615	2557	14
H2B	13170	9683	1307	14
H7A	10942	4552	1300	16
H7B	12059	4778	143	16
H14A	12127	5644	3866	26
H14B	13235	5974	4801	26
H14C	14022	6280	3589	26
H4	11492	8358	437	12
H3	13217	7855	1964	12
H10	14796	1462	1006	21
H5	10797	6646	107	13
H13	15225	5097	1872	18
H1A	10054	9999	2888	16
H1B	11202	10963	2245	16
H9	12564	2693	594	17
H11	17221	2031	1894	25
H18A	9246	8998	5559	28
H18B	7282	8431	5757	28
H18C	8177	8785	4575	28
H17A	10296	6222	6189	31
H17B	8552	6854	6736	31
H17C	10519	7418	6567	31
H15A	12608	9234	4731	28
H15B	14334	8609	4152	28
H15C	13545	8303	5364	28
H16A	8602	5898	4592	31
H16B	7785	6893	3983	31
H16C	6888	6538	5165	31
H12	17430	3855	2313	24

References:

[6] BRUKER-AXS. (2007-2013) APEX2 (Ver. 2013.2-0), SADABS (2012-1)

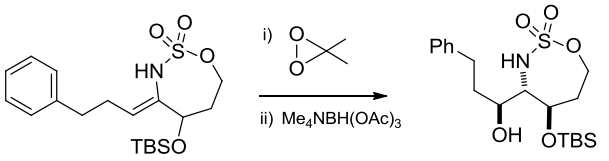
[7] SAINT+ (Ver. 8.30C) Software Reference Manuals, BRUKER-AXS, Madison, Wisconsin, USA.

[8] G. M. Sheldrick, *Acta Cryst.*, **2008**, *A64*, 112-122.

[9] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. L. Howard, H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339-341.

[10] XP – X-Ray Crystal Structure Visualization BRUKER, AXS, **1998**, V5.1

<u>Crystal Structure of Schomaker30</u> [CSA4199]



[41] = [CSA4199]

Preparation of Crystals: The racemic compound (CSA4199) was dissolved in a mixture n-hexane / ethyl acetate and crystallized at room temperature by slow vapor diffusion. The obtained crystals were air-stable and selected under microscope.

Data Collection: A colorless crystal with approximate dimensions 0.229 x 0.157 x 0.129 mm^3 (block) was selected under oil under ambient conditions and attached to the tip of a X-ray capillary (MiTeGenMicroMount©). The crystal was mounted in a stream of cold nitrogen at 200.0(15) K and centered in the X-ray beam by using a video camera. The crystal evaluation and data collection were performed on a three-circle Bruker Quazar SMART APEXII diffractometer with Molybdenum K_α(λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 4.96 cm. The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 12 frames collected at intervals of 0.5° in 6° range about ω with the exposure time of 10 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEXII program suite. The final cell constants were calculated from a set of 9172 strong from the actual data collection. The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.70 Å. A total of 54259 reflection data were harvested by collecting 6 sets of frames with 0.6° scans in ω and φ with exposure times of 25 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [11,12]

Structure Solution and Refinement: The systematic absences in the diffraction data were consistent for the triclinic space groups P1 and $P\bar{1}$. The *E*-statistics strongly suggested the centrosymmetric space group that yielded chemically reasonable and computationally stable results of refinement. [13,14] A successful solution by the "direct methods" by using SHELX-2013 provided most non-hydrogen atoms from the *E*-map. Using Olex2, all non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. The severe disorder in the TBS-protecting group (Si1A) in the second molecule of the unit was modeled with 3 components in A:B:C in three ways with restraints and constraints. Crystal diffraction data outlier elimination was carried out using "G4 - FCF filter". [16]

Table 16. Crystal data collection and structure solution refinement for Schomaker30 [CSA4099]

Parameter	CSA4099	Parameter	CSA4099
empiric formula	$C_{19}H_{33}NO_5SSi$	$\rho_{calc.}$ [g · cm^{-1}]	1.204
MW [g · mol^{-1}]	416.12	crystal size [mm]	0.229 × 0.157 × 0.129
X-ray lab code	Schomaker30	T [K]	200.0(15)
a [Å]	11.8101(17)	radiation type / λ [nm]	Mo K_α / 0.71072
b [Å]	12.7217(17)	μ [mm^{-1}]	0.220
c [Å]	16.841(2)	F(000)	898.0
α [°]	72.829(6)	Reflections collected	54072
β [°]	75.377(7)	Independent reflections	11307 [R_{int} = 0.0266]
γ [°]	75.493(6)	Data/restraints/parameters	11307/379/646
V [Å^3]	2296.4(6)	GooF on F^2	1.022
Z	2	Largest diff. peak/hole [eÅ^{-3}]	0.34 / -0.31
crystal system	triclinic		
crystal color	colorless	Final R_1[a]/ wR_2[b] all data	0.0433/ 0.1006
space group	$P\bar{1}$	Final R_1[a]/ wR_2[b] I>2s(I)	0.0367/ 0.0956

[a] $R_1 = \sum| F_o| - | F_c| / | F_o|$;[b] $wR_2 = [\sum\{w(F_o^2 - F_o^2)^2\}/ \sum\{w(F_o^2)^2\}]^{1/2}$

The final least-squares refinement of 646 parameters against 11307 data resulted in R = 0.0357 (based on F^2 for I>2s) and wR2 = 0.01006 (based on F^2 for all data), respectively. The final structure was visualized using Interactive Molecular Graphics. [15]

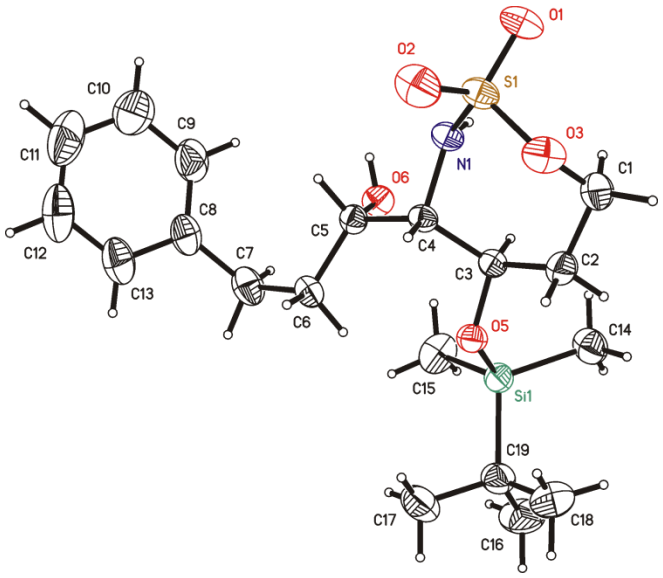


Figure 3. Thermal-ellipsoid of Schomaker30 [CSA4199] are set with 50 % probability

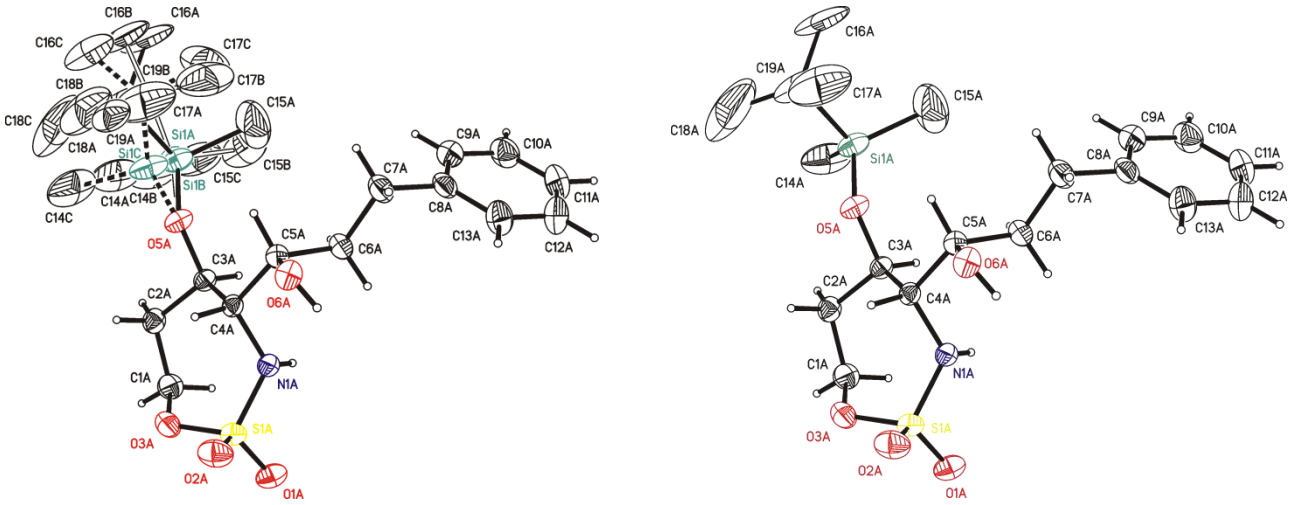


Figure 4. Thermal-ellipsoid of the disordered molecule (left) of Schomaker30 [CSA4199] are set with 50 % probability. The disorder parts Si1B and Si1C of the protecting group were omitted for more clarity (right).

Table 17. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for Schomaker30 [CSA4099]. U_{eq} is defined as 1/3 of of the trace of the orthogonalized U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Si1	1272.6(3)	-775.7(3)	6990.2(2)	31.60(9)
O3	4474.8(9)	2308.5(9)	5170.4(7)	40.0(2)
C14	885.7(16)	-497.0(14)	5927.4(10)	46.4(4)
C15	-100.0(15)	-304.2(16)	7722.9(12)	51.4(4)
C16	1064(2)	-3034.4(16)	7459.9(15)	63.7(5)
C17	2258(2)	-2484.4(16)	8252.1(12)	62.2(5)
C18	3101.0(19)	-2616.6(16)	6764.7(14)	60.6(5)
C19	1951.1(15)	-2290.8(12)	7383.3(10)	41.0(3)
S1	3771.1(3)	3314.2(3)	5568.2(2)	31.29(8)
O1	3343.6(9)	4237.2(8)	4922.7(7)	39.9(2)
O2	4571.2(10)	3446.6(10)	6018.4(8)	48.6(3)
O5	2333.7(8)	-86.6(7)	6921.9(6)	30.19(19)
O6	672.0(8)	2214.9(8)	7471.1(6)	32.3(2)
N1	2627.6(10)	2884.6(9)	6198.0(7)	27.9(2)
C1	3753.8(15)	1750.6(13)	4891.5(9)	40.9(3)
C2	3413.5(14)	754.2(12)	5591.0(9)	35.8(3)
C3	2442.2(11)	977(1)	6352.9(8)	27.0(2)
C4	2717.4(11)	1762.1(10)	6796.7(8)	25.2(2)
C5	1859.5(11)	1929(1)	7622.5(8)	26.9(2)
C6	1956.5(13)	947.8(12)	8400.6(8)	33.3(3)

C7	1030.9(15)	1178.0(15)	9185.0(9)	44.1(4)
C8	1206.6(14)	2084.5(15)	9528.2(9)	42.9(3)
C9	825.3(18)	3213.3(17)	9178.6(11)	56.1(5)
C10	1030(2)	4032(2)	9490.2(14)	75.4(7)
C11	1595(2)	3733(2)	10168.7(15)	79.8(7)
C12	1956(2)	2628(2)	10531.7(13)	71.2(6)
C13	1778.7(17)	1809.1(19)	10212.1(11)	55.5(4)
Si1A	-4337(14)	3095(10)	8474(9)	35.0(14)
C14A	-5584(9)	2685(12)	8236(6)	76(3)
C15A	-4898(12)	4542(8)	8601(10)	109(5)
C16A	-4942(14)	2700(12)	10184(7)	102(4)
C17A	-2702(10)	2458(14)	9548(6)	102(3)
C18A	-3752(15)	980(9)	9475(9)	172(7)
C19A	-3913(10)	2194(10)	9508(7)	84(3)
S1A	-614.2(3)	3519.6(3)	5111.43(19)	26.89(8)
O1A	-807.0(9)	4180.9(9)	4292.0(6)	35.7(2)
O2A	577.3(9)	3083.9(9)	5240.9(6)	38.5(2)
O3A	-1183.5(9)	2452.1(8)	5348.9(6)	34.9(2)
O5A	-3116.6(8)	2962.4(8)	7798.9(5)	30.48(19)
O6A	-309.5(8)	4452.0(7)	7155.7(6)	28.57(19)
N1A	-1353.6(10)	4244.0(8)	5772.6(6)	23.7(2)
C1A	-2496.1(13)	2623.7(11)	5569.3(8)	32.3(3)
C2A	-2892.2(12)	2420.4(10)	6517.7(8)	28.4(3)
C3A	-2872.6(11)	3359.1(10)	6905.6(7)	23.5(2)
C4A	-1645.5(10)	3693.5(9)	6680.9(7)	21.4(2)
C5A	-1537.7(11)	4453.2(9)	7206.6(7)	23.4(2)
C6A	-2236.7(12)	5644.5(10)	6969.8(8)	27.2(2)
C7A	-2275.7(14)	6319.8(11)	7596.8(9)	34.9(3)
C8A	-2840.9(13)	7534.9(11)	7303.4(8)	31.2(3)
C9A	-4055.4(14)	7913.8(12)	7516.5(10)	39.5(3)
C10A	-4565.2(15)	9030.9(13)	7234.4(11)	44.6(4)
C11A	-3858.4(15)	9782.8(12)	6727.4(11)	44.5(4)
C12A	-2650.5(15)	9419.0(13)	6497.5(12)	46.3(4)
C13A	-2143.6(14)	8300.3(12)	6780.9(11)	40.4(3)
Si1B	-4409(10)	3011(7)	8510(7)	32.2(11)
C14B	-5217(8)	2005(10)	8403(5)	84(3)
C15B	-5307(8)	4426(8)	8243(5)	98(4)
C16B	-4873(10)	2279(11)	10303(6)	99(3)
C17B	-3277(10)	3535(9)	9559(4)	102(3)
C18B	-3015(10)	1477(9)	9626(5)	112(3)
C19B	-3873(8)	2609(7)	9514(6)	56.2(16)
Si1C	-4274(4)	2560(5)	8498(2)	46.7(10)
C14C	-4455(15)	1151(12)	8498(8)	107(5)
C15C	-5622(8)	3570(14)	8250(6)	90(4)
C16C	-4570(12)	1652(13)	10258(7)	89(3)
C17C	-4095(14)	3628(10)	9697(8)	93(3)
C18C	-2556(9)	1878(9)	9512(7)	54(2)
C19C	-3865(14)	2481(12)	9517(8)	73(3)

Table 18. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Schomaker30 [CSA4099]. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	34.4(2)	31.44(18)	31.23(18)	-6.90(14)	-8.06(15)	-9.67(14)
O3	26.8(5)	37.1(5)	47.3(6)	-6.1(4)	0.3(4)	-3.0(4)
C14	54(1)	48.9(9)	44.4(8)	-5.9(7)	-21.1(7)	-19.0(7)
C15	38.2(9)	59.5(10)	60.5(10)	-24.2(8)	2.5(7)	-17.6(7)
C16	77.2(14)	41.3(9)	81.2(14)	-5.3(9)	-27.2(11)	-26.4(9)
C17	89.2(15)	49.8(10)	50(1)	2.1(8)	-34.7(10)	-13.4(10)
C18	63.9(12)	44.3(9)	68.6(12)	-16.9(9)	-15.3(10)	4.9(8)
C19	51.6(9)	33.4(7)	41.4(8)	-4.4(6)	-15.7(7)	-13.0(6)
S1	25.66(16)	30.04(16)	34.81(17)	0.34(12)	-9.95(13)	-5.20(12)
O1	34.5(5)	34.5(5)	41.1(6)	6.6(4)	-10.3(4)	-5.5(4)
O2	40.9(6)	55.1(7)	54.2(7)	-1.2(5)	-21.5(5)	-19.4(5)
O5	33.3(5)	26.8(4)	31.0(5)	-4.4(3)	-9.1(4)	-6.9(4)
O6	24.5(5)	33.4(5)	38.7(5)	-9.8(4)	-9.7(4)	-0.1(4)
N1	24.4(6)	26.7(5)	29.7(5)	-2.2(4)	-8.8(4)	-2.0(4)
C1	46.2(9)	41.8(8)	30.3(7)	-10.0(6)	1.4(6)	-8.0(6)
C2	40.2(8)	33.6(7)	32.0(7)	-11.5(5)	-1.4(6)	-5.7(6)
C3	28.1(6)	26.2(6)	26.2(6)	-5.2(4)	-7.3(5)	-3.5(5)
C4	23.4(6)	24.3(5)	26.9(6)	-3.7(4)	-8.8(5)	-1.8(4)
C5	25.0(6)	28.7(6)	27.5(6)	-7.5(5)	-7.7(5)	-2.8(5)
C6	37.4(7)	34.9(7)	26.9(6)	-4.4(5)	-10.0(5)	-5.6(5)
C7	43.2(9)	56.3(9)	30.1(7)	-4.7(6)	-2.9(6)	-16.0(7)
C8	38.0(8)	61(1)	25.4(6)	-13.3(6)	3.9(6)	-8.7(7)
C9	61.4(11)	64.1(11)	36.8(8)	-21.9(8)	-4.7(8)	4.9(9)
C10	99.2(18)	64.5(13)	55.3(12)	-30.8(10)	1.7(11)	-0.4(12)
C11	93.3(18)	98.3(19)	61.5(13)	-50.4(13)	0.4(12)	-21.5(14)
C12	67.6(14)	111.3(19)	45.4(10)	-40.6(12)	-8.2(9)	-13.7(13)
C13	55.3(11)	77.5(13)	31.6(8)	-16.3(8)	-5.1(7)	-8.9(9)
Si1A	28(2)	49(3)	24.7(18)	-3.3(17)	-0.7(15)	-12.8(18)
C14A	50(5)	139(8)	52(4)	-28(6)	4(3)	-51(6)
C15A	88(8)	58(5)	148(12)	-39(6)	43(7)	-5(5)
C16A	110(6)	144(8)	18(4)	10(5)	6(4)	-17(6)
C17A	85(5)	165(8)	49(4)	-5(6)	-39(4)	-12(6)
C18A	156(10)	129(9)	124(9)	72(7)	0(8)	16(8)
C19A	56(4)	125(6)	32(3)	13(4)	1(3)	2(4)
S1A	25.76(16)	31.28(15)	23.00(14)	-7.96(11)	-3.14(11)	-4.41(11)
O1A	36.5(5)	47.1(6)	23.0(4)	-5.3(4)	-4.9(4)	-11.8(4)
O2A	26.0(5)	50.1(6)	36.7(5)	-14.4(4)	-4.9(4)	0.8(4)
O3A	38.0(5)	29.5(5)	37.8(5)	-14.7(4)	-1.1(4)	-6.2(4)
O5A	30.4(5)	39.1(5)	21.6(4)	-3.1(4)	-3.5(3)	-12.8(4)
O6A	26.2(5)	29.4(4)	31.4(5)	-3.6(3)	-11.2(4)	-6.8(3)
N1A	25.7(5)	22.0(5)	21.5(5)	-3.6(4)	-5.0(4)	-3.1(4)
C1A	36.8(7)	34.3(6)	31.9(6)	-11.6(5)	-6.5(5)	-13.4(5)
C2A	31.0(7)	27.1(6)	29.7(6)	-6.0(5)	-6.8(5)	-10.5(5)
C3A	24.3(6)	24.9(5)	21.2(5)	-3.9(4)	-5.8(4)	-5.3(4)
C4A	23.1(6)	19.9(5)	20.4(5)	-3.1(4)	-5.8(4)	-3.3(4)
C5A	24.1(6)	23.3(5)	23.7(5)	-5.4(4)	-6.6(4)	-4.5(4)

C6A	29.5(6)	23.9(5)	30.2(6)	-9.5(5)	-9.6(5)	-1.8(5)
C7A	48.5(8)	26.5(6)	33.8(7)	-11.2(5)	-14.8(6)	-2.8(5)
C8A	41.5(8)	26.8(6)	30.9(6)	-13.1(5)	-11.2(5)	-4.8(5)
C9A	43.3(8)	35.5(7)	38.0(7)	-11.4(6)	-0.6(6)	-9.0(6)
C10A	38.3(8)	39.3(8)	53.3(9)	-18.5(7)	-3.4(7)	0.9(6)
C11A	49.1(9)	27.4(6)	61.2(10)	-14.1(6)	-19.4(8)	-2.1(6)
C12A	48.1(9)	31.0(7)	62.2(10)	-5.9(7)	-14.9(8)	-14.4(6)
C13A	34.3(8)	33.1(7)	56.1(9)	-12.3(6)	-11.1(7)	-7.0(6)
Si1B	27.2(16)	39(2)	26.4(15)	-2.1(14)	0.1(11)	-11.6(14)
C14B	78(6)	138(7)	58(4)	-28(5)	15(4)	-82(5)
C15B	71(6)	92(6)	70(4)	5(4)	10(3)	42(5)
C16B	90(5)	134(8)	25(4)	21(5)	9(3)	-6(6)
C17B	129(6)	157(6)	47(3)	-30(4)	-16(4)	-73(5)
C18B	94(6)	125(7)	69(4)	30(4)	-24(4)	11(5)
C19B	57(3)	92(4)	22(2)	-6(2)	-6(2)	-29(3)
Si1C	41.7(16)	77(3)	24.0(9)	-8.6(16)	0.5(9)	-28.5(19)
C14C	156(12)	129(9)	64(6)	-18(7)	15(7)	-119(9)
C15C	52(5)	129(8)	54(5)	-3(6)	3(4)	6(6)
C16C	83(6)	121(8)	39(4)	13(6)	-6(4)	-23(6)
C17C	112(7)	108(7)	71(5)	-51(5)	-29(6)	5(6)
C18C	54(5)	63(5)	34(4)	1(4)	-19(3)	2(4)
C19C	64(5)	110(5)	31(4)	-4(5)	-4(4)	-16(5)

Table 19. Bond Lengths for Schomaker30 [CSA4099]

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Si1	C14	1.8696(16)	S1A	O1A	1.4287(10)
Si1	C15	1.8574(17)	S1A	O2A	1.4240(10)
Si1	C19	1.8805(16)	S1A	O3A	1.5676(10)
Si1	O5	1.6643(10)	S1A	N1A	1.6010(11)
O3	S1	1.5711(11)	O3A	C1A	1.4752(17)
O3	C1	1.4668(19)	O5A	C3A	1.4165(14)
C16	C19	1.538(2)	O5A	Si1B	1.686(13)
C17	C19	1.531(2)	O5A	Si1C	1.642(4)
C18	C19	1.536(3)	O6A	C5A	1.4309(15)
S1	O1	1.4289(10)	N1A	C4A	1.4735(15)
S1	O2	1.4188(11)	C1A	C2A	1.5086(18)
S1	N1	1.5975(12)	C2A	C3A	1.5282(16)
O5	C3	1.4230(15)	C3A	C4A	1.5367(16)
O6	C5	1.4263(15)	C4A	C5A	1.5356(15)
N1	C4	1.4816(15)	C5A	C6A	1.5231(16)
C1	C2	1.513(2)	C6A	C7A	1.5319(17)
C2	C3	1.5334(18)	C7A	C8A	1.5092(18)
C3	C4	1.5452(17)	C8A	C9A	1.384(2)
C4	C5	1.5365(17)	C8A	C13A	1.389(2)
C5	C6	1.5254(18)	C9A	C10A	1.388(2)
C6	C7	1.538(2)	C10A	C11A	1.378(2)
C7	C8	1.510(2)	C11A	C12A	1.377(2)
C8	C9	1.386(3)	C12A	C13A	1.388(2)

C8	C13	1.394(2)	Si1B	C14B	1.848(9)
C9	C10	1.390(3)	Si1B	C15B	1.837(9)
C10	C11	1.378(4)	Si1B	C19B	1.841(9)
C11	C12	1.362(4)	C16B	C19B	1.569(10)
C12	C13	1.385(3)	C17B	C19B	1.544(9)
Si1A	C14A	1.845(12)	C18B	C19B	1.530(10)
Si1A	C15A	1.850(12)	Si1C	C14C	1.858(10)
Si1A	C19A	1.889(11)	Si1C	C15C	1.831(10)
Si1A	O5A	1.601(17)	Si1C	C19C	1.865(11)
C16A	C19A	1.590(12)	C16C	C19C	1.581(13)
C17A	C19A	1.570(13)	C17C	C19C	1.523(13)
C18A	C19A	1.524(13)	C18C	C19C	1.543(14)

Table 20. Bond Angles for Schomaker30 [CSA4099]

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C14	Si1	C19	111.58(7)	O2A	S1A	O3A	103.98(6)
C15	Si1	C14	107.86(9)	O2A	S1A	N1A	111.25(6)
C15	Si1	C19	112.58(8)	O3A	S1A	N1A	106.00(5)
O5	Si1	C14	110.18(6)	C1A	O3A	S1A	116.79(8)
O5	Si1	C15	110.42(7)	Si1A	O5A	Si1B	4.0(7)
O5	Si1	C19	104.20(6)	Si1A	O5A	Si1C	23.3(5)
C1	O3	S1	115.81(9)	C3A	O5A	Si1A	131.0(4)
C16	C19	Si1	109.78(12)	C3A	O5A	Si1B	131.5(3)
C17	C19	Si1	110.01(12)	C3A	O5A	Si1C	134.30(16)
C17	C19	C16	109.16(15)	Si1C	O5A	Si1B	19.3(3)
C17	C19	C18	108.55(16)	C4A	N1A	S1A	120.13(8)
C18	C19	Si1	109.96(11)	O3A	C1A	C2A	109.48(11)
C18	C19	C16	109.35(15)	C1A	C2A	C3A	116.47(10)
O3	S1	N1	105.16(6)	O5A	C3A	C2A	108.27(9)
O1	S1	O3	109.57(7)	O5A	C3A	C4A	105.79(9)
O1	S1	N1	106.87(6)	C2A	C3A	C4A	112.95(10)
O2	S1	O3	103.65(7)	N1A	C4A	C3A	110.81(9)
O2	S1	O1	119.37(7)	N1A	C4A	C5A	109.44(9)
O2	S1	N1	111.35(7)	C5A	C4A	C3A	113.47(10)
C3	O5	Si1	123.56(8)	O6A	C5A	C4A	110.09(9)
C4	N1	S1	121.88(9)	O6A	C5A	C6A	111.00(9)
O3	C1	C2	109.85(12)	C6A	C5A	C4A	113.70(9)
C1	C2	C3	118.18(12)	C5A	C6A	C7A	112.15(10)
O5	C3	C2	106.55(10)	C8A	C7A	C6A	111.84(11)
O5	C3	C4	110.79(10)	C9A	C8A	C7A	121.82(13)
C2	C3	C4	113.25(11)	C9A	C8A	C13A	118.15(13)
N1	C4	C3	106.31(10)	C13A	C8A	C7A	120.00(13)
N1	C4	C5	105.70(10)	C8A	C9A	C10A	121.22(14)
C5	C4	C3	116.67(10)	C11A	C10A	C9A	119.89(15)
O6	C5	C4	108.16(10)	C12A	C11A	C10A	119.77(14)
O6	C5	C6	109.79(11)	C11A	C12A	C13A	120.17(15)
C6	C5	C4	116.31(10)	C12A	C13A	C8A	120.78(15)
C5	C6	C7	112.39(12)	O5A	Si1B	C14B	108.0(6)

C8	C7	C6	115.05(13)	O5A	Si1B	C15B	108.2(6)
C9	C8	C7	122.17(15)	O5A	Si1B	C19B	101.6(6)
C9	C8	C13	117.26(17)	C15B	Si1B	C14B	108.4(7)
C13	C8	C7	120.56(17)	C15B	Si1B	C19B	116.1(6)
C8	C9	C10	121.03(19)	C19B	Si1B	C14B	114.0(6)
C11	C10	C9	120.3(2)	C16B	C19B	Si1B	112.3(7)
C12	C11	C10	119.5(2)	C17B	C19B	Si1B	109.6(6)
C11	C12	C13	120.4(2)	C17B	C19B	C16B	113.9(8)
C12	C13	C8	121.4(2)	C18B	C19B	Si1B	112.0(7)
C14A	Si1A	C15A	105.7(9)	C18B	C19B	C16B	97.8(7)
C14A	Si1A	C19A	112.1(9)	C18B	C19B	C17B	110.8(8)
C15A	Si1A	C19A	107.3(9)	O5A	Si1C	C14C	112.4(5)
O5A	Si1A	C14A	114.7(8)	O5A	Si1C	C15C	108.9(5)
O5A	Si1A	C15A	113.4(8)	O5A	Si1C	C19C	102.1(5)
O5A	Si1A	C19A	103.6(7)	C14C	Si1C	C19C	109.1(6)
C16A	C19A	Si1A	101.9(9)	C15C	Si1C	C14C	108.4(7)
C17A	C19A	Si1A	107.0(8)	C15C	Si1C	C19C	116.0(7)
C17A	C19A	C16A	108.7(11)	C16C	C19C	Si1C	109.0(9)
C18A	C19A	Si1A	106.6(9)	C17C	C19C	Si1C	112.3(8)
C18A	C19A	C16A	120.9(11)	C17C	C19C	C16C	111.3(12)
C18A	C19A	C17A	110.5(10)	C17C	C19C	C18C	111.9(11)
O1A	S1A	O3A	109.34(6)	C18C	C19C	Si1C	109.4(9)
O1A	S1A	N1A	106.71(6)	C18C	C19C	C16C	102.5(10)
O2A	S1A	O1A	118.87(6)				

Table 21. Torsion Angles for Schomaker30 [CSA4099]

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Si1	O5	C3	C2	-99.48(11)	S1A	O3A	C1A	C2A	-94.68(11)
Si1	O5	C3	C4	136.93(9)	S1A	N1A	C4A	C3A	-92.51(11)
O3	S1	N1	C4	46.01(11)	S1A	N1A	C4A	C5A	141.62(9)
O3	C1	C2	C3	74.69(17)	O1A	S1A	O3A	C1A	-72.91(10)
C14	Si1	C19	C16	-60.01(15)	O1A	S1A	N1A	C4A	161.42(9)
C14	Si1	C19	C17	179.84(13)	O2A	S1A	O3A	C1A	159.16(9)
C14	Si1	C19	C18	60.33(14)	O2A	S1A	N1A	C4A	-67.46(11)
C14	Si1	O5	C3	33.39(12)	O3A	S1A	N1A	C4A	44.95(10)
C15	Si1	C19	C16	61.44(15)	O3A	C1A	C2A	C3A	77.53(14)
C15	Si1	C19	C17	-58.71(15)	O5A	Si1A	C19A	C16A	158.7(10)
C15	Si1	C19	C18	-178.21(12)	O5A	Si1A	C19A	C17A	44.7(10)
C15	Si1	O5	C3	-85.66(12)	O5A	Si1A	C19A	C18A	-73.6(10)
C19	Si1	O5	C3	153.21(10)	O5A	C3A	C4A	N1A	-173.41(9)
S1	O3	C1	C2	-93.78(13)	O5A	C3A	C4A	C5A	-49.82(12)
S1	N1	C4	C3	-95.24(11)	O5A	Si1B	C19B	C16B	-165.0(7)
S1	N1	C4	C5	140.14(9)	O5A	Si1B	C19B	C17B	67.3(8)
O1	S1	N1	C4	162.41(10)	O5A	Si1B	C19B	C18B	-56.0(8)
O2	S1	N1	C4	-65.61(12)	O5A	Si1C	C19C	C16C	-156.6(8)
O5	Si1	C19	C16	-178.88(12)	O5A	Si1C	C19C	C17C	79.7(11)
O5	Si1	C19	C17	60.97(14)	O5A	Si1C	C19C	C18C	-45.3(10)
O5	Si1	C19	C18	-58.54(13)	O6A	C5A	C6A	C7A	-64.53(14)

O5	C3	C4	N1	-171.50(10)	N1A	S1A	O3A	C1A	41.78(10)
O5	C3	C4	C5	-53.95(14)	N1A	C4A	C5A	O6A	-73.16(11)
O6	C5	C6	C7	-54.60(15)	N1A	C4A	C5A	C6A	52.10(13)
N1	C4	C5	O6	67.49(12)	C1A	C2A	C3A	O5A	-172.37(11)
N1	C4	C5	C6	-168.49(11)	C1A	C2A	C3A	C4A	-55.56(15)
C1	O3	S1	O1	-69.91(11)	C2A	C3A	C4A	N1A	68.32(12)
C1	O3	S1	O2	161.63(10)	C2A	C3A	C4A	C5A	-168.09(10)
C1	O3	S1	N1	44.63(11)	C3A	O5A	Si1B	C14B	72.4(6)
C1	C2	C3	O5	-177.75(12)	C3A	O5A	Si1B	C15B	-44.7(7)
C1	C2	C3	C4	-55.70(17)	C3A	O5A	Si1B	C19B	-167.4(3)
C2	C3	C4	N1	68.85(13)	C3A	O5A	Si1C	C14C	74.8(6)
C2	C3	C4	C5	-173.60(10)	C3A	O5A	Si1C	C15C	-45.3(7)
C3	C4	C5	O6	-50.39(13)	C3A	O5A	Si1C	C19C	-168.4(5)
C3	C4	C5	C6	73.64(14)	C3A	C4A	C5A	O6A	162.50(9)
C4	C5	C6	C7	-177.78(11)	C3A	C4A	C5A	C6A	-72.24(13)
C5	C6	C7	C8	-67.35(17)	C4A	C5A	C6A	C7A	170.69(11)
C6	C7	C8	C9	81.2(2)	C5A	C6A	C7A	C8A	173.20(12)
C6	C7	C8	C13	-98.08(18)	C6A	C7A	C8A	C9A	89.45(16)
C7	C8	C9	C10	-178.05(18)	C6A	C7A	C8A	C13A	-88.31(16)
C7	C8	C13	C12	179.51(17)	C7A	C8A	C9A	C10A	-179.25(14)
C8	C9	C10	C11	-1.5(3)	C7A	C8A	C13A	C12A	179.30(14)
C9	C8	C13	C12	0.2(3)	C8A	C9A	C10A	C11A	0.5(2)
C9	C10	C11	C12	0.2(4)	C9A	C8A	C13A	C12A	1.5(2)
C10	C11	C12	C13	1.3(4)	C9A	C10A	C11A	C12A	0.6(3)
C11	C12	C13	C8	-1.5(3)	C10A	C11A	C12A	C13A	-0.5(3)
C13	C8	C9	C10	1.2(3)	C11A	C12A	C13A	C8A	-0.5(3)
Si1A	O5A	C3A	C2A	-95.9(6)	C13A	C8A	C9A	C10A	-1.5(2)
Si1A	O5A	C3A	C4A	142.8(6)	Si1B	O5A	C3A	C2A	-90.6(4)
Si1A	O5A	Si1B	C14B	157(9)	Si1B	O5A	C3A	C4A	148.1(4)
Si1A	O5A	Si1B	C15B	40(9)	Si1B	O5A	Si1C	C14C	165.6(11)
Si1A	O5A	Si1B	C19B	-83(9)	Si1B	O5A	Si1C	C15C	45.5(10)
Si1A	O5A	Si1C	C14C	167.6(13)	Si1B	O5A	Si1C	C19C	-77.7(10)
Si1A	O5A	Si1C	C15C	47.5(12)	C14B	Si1B	C19B	C16B	-49.1(11)
Si1A	O5A	Si1C	C19C	-75.6(12)	C14B	Si1B	C19B	C17B	-176.8(8)
C14A	Si1A	C19A	C16A	-77.1(13)	C14B	Si1B	C19B	C18B	59.8(11)
C14A	Si1A	C19A	C17A	168.9(10)	C15B	Si1B	C19B	C16B	77.9(10)
C14A	Si1A	C19A	C18A	50.6(13)	C15B	Si1B	C19B	C17B	-49.8(11)
C14A	Si1A	O5A	C3A	51.8(10)	C15B	Si1B	C19B	C18B	-173.2(9)
C14A	Si1A	O5A	Si1B	-47(9)	Si1C	O5A	C3A	C2A	-64.4(4)
C14A	Si1A	O5A	Si1C	-57.0(11)	Si1C	O5A	C3A	C4A	174.3(3)
C15A	Si1A	C19A	C16A	38.6(13)	Si1C	O5A	Si1B	C14B	-34.8(8)
C15A	Si1A	C19A	C17A	-75.5(12)	Si1C	O5A	Si1B	C15B	-152.0(12)
C15A	Si1A	C19A	C18A	166.2(10)	Si1C	O5A	Si1B	C19B	85.3(9)
C15A	Si1A	O5A	C3A	-69.7(9)	C14C	Si1C	C19C	C16C	-37.4(12)
C15A	Si1A	O5A	Si1B	-169(10)	C14C	Si1C	C19C	C17C	-161.2(11)
C15A	Si1A	O5A	Si1C	-178.6(16)	C14C	Si1C	C19C	C18C	73.9(11)
C19A	Si1A	O5A	C3A	174.3(4)	C15C	Si1C	C19C	C16C	85.2(11)
C19A	Si1A	O5A	Si1B	75(9)	C15C	Si1C	C19C	C17C	-38.5(14)

C19A Si1A O5A Si1C 65.5(11) C15C Si1C C19C C18C -163.4(9)

Table 22. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for Schomaker30

Atom	*x*	*y*	*z*	U(eq)
H14J	289	-935	5970	70
H14K	1604	-713	5523	70
H14L	562	303	5733	70
H15J	-336	513	7547	77
H15K	55	-523	8300	77
H15L	-743	-654	7708	77
H16J	338	-2841	7866	96
H16K	1426	-3823	7658	96
H16L	864	-2913	6905	96
H17J	2806	-1997	8210	93
H17K	2638	-3269	8443	93
H17L	1527	-2311	8660	93
H18J	2915	-2515	6209	91
H18K	3457	-3403	6979	91
H18L	3665	-2140	6712	91
H6	438	2912	7383	49
H1B	4213	1497	4380	49
H1C	3025	2285	4744	49
H2A	4142	319	5807	43
H2B	3152	269	5335	43
H3	1671	1324	6155	32
H4	3550	1494	6904	30
H5	2021	2588	7755	32
H6B	2766	793	8525	40
H6C	1844	271	8276	40
H7A	229	1390	9040	53
H7B	1050	475	9639	53
H9	418	3431	8719	67
H10	778	4802	9234	90
H11	1733	4294	10382	96
H12	2332	2419	11007	85
H13	2053	1043	10464	67
H14A	-6252	2675	8719	114
H14B	-5323	1937	8128	114
H14C	-5838	3226	7734	114
H15A	-5069	5044	8061	163
H15B	-4292	4785	8774	163
H15C	-5628	4563	9034	163
H16A	-5210	3501	9945	153
H16B	-4636	2601	10696	153
H16C	-5613	2311	10327	153
H17A	-2046	2065	9190	153
H17B	-2580	2206	10134	153

H17C	-2724	3267	9343	153
H18A	-4535	790	9555	259
H18B	-3339	486	9926	259
H18C	-3279	884	8924	259
H6A	-43	4857	6685	43
H1AA	-2780	2101	5364	39
H1AB	-2843	3399	5293	39
H2AA	-2376	1731	6784	34
H2AB	-3715	2276	6669	34
H3A	-3490	4029	6723	28
H4A	-1037	2990	6797	26
H5A	-1874	4120	7811	28
H6AA	-3061	5617	6954	33
H6AB	-1865	6028	6396	33
H7AA	-2734	5990	8156	42
H7AB	-1454	6271	7665	42
H9A	-4549	7399	7862	47
H10A	-5400	9277	7390	54
H11A	-4203	10550	6537	53
H12A	-2162	9935	6144	56
H13A	-1310	8055	6616	48
H14D	-5395	2226	7832	126
H14E	-5964	2003	8821	126
H14F	-4722	1253	8498	126
H15D	-4865	4977	8256	148
H15E	-6058	4476	8657	148
H15F	-5478	4582	7676	148
H16D	-5441	2956	10403	148
H16E	-4512	1901	10803	148
H16F	-5290	1774	10196	148
H17D	-2445	3423	9262	153
H17E	-3306	3500	10152	153
H17F	-3702	4270	9290	153
H18D	-3329	945	9461	169
H18E	-2934	1189	10221	169
H18F	-2234	1570	9269	169
H14G	-4654	1184	7959	161
H14H	-5098	911	8965	161
H14I	-3710	614	8570	161
H15G	-5608	4286	8350	134
H15H	-6326	3284	8612	134
H15I	-5653	3679	7654	134
H16G	-5376	1744	10158	133
H16H	-4619	1819	10799	133
H16I	-4152	878	10275	133
H17G	-4030	4204	9161	140
H17H	-3506	3642	10010	140
H17I	-4898	3776	10036	140
H18G	-2408	1211	9295	81

H18H	-2404	1654	10090	81
H18I	-2026	2385	9148	81
H1	2064(17)	3094(15)	5992(12)	43(5)
H1A	-1897(15)	4737(14)	5580(10)	31(4)

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