

Supporting Information for

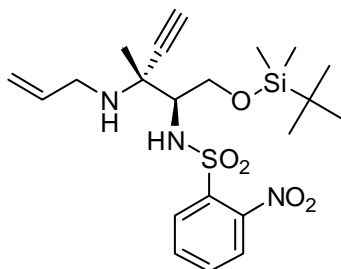
Ring-Opening of a Trisubstituted Aziridine with Amines: Regio- and Stereoselective Formation of Substituted 1,2-Diamines

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X-ray Structure Determination of Compound 2a



Compound **2a**, C₂₁H₃₃SiN₃SO₅, crystallizes in the monoclinic space group P2₁ (systematic absences 0k0: k=odd) with a=7.6795(2)Å, b=8.1287(2)Å, c=21.2564(5)Å, β=99.9650(10)°, V=1306.90(6)Å³, Z=2, and d_{calc}=1.188 g/cm³. X-ray intensity data were collected on a Bruker APEXII CCD area detector employing graphite-monochromated Mo-Kα radiation (λ=0.71073 Å) at a temperature of 143(1)K. Preliminary indexing was performed from a series of thirty-six 0.5° rotation frames with exposures of 20 seconds. A total of 1606 frames were collected with a crystal to detector distance of 37.560 mm, rotation widths of 0.5° and exposures of 20 seconds:

scan type	2θ	ω	φ	χ	frames
φ	19.50	59.55	-10.95	-26.26	738
ω	-20.50	-16.03	-181.36	-31.86	129
φ	-10.50	300.13	-342.23	39.97	739

Rotation frames were integrated using SAINTⁱ, producing a listing of unaveraged F² and σ(F²) values which were then passed to the SHELXTLⁱⁱ program package for further processing

and structure solution on a Dell Pentium 4 computer. A total of 17678 reflections were measured over the ranges $1.95 \leq \theta \leq 25.05^\circ$, $-9 \leq h \leq 9$, $-9 \leq k \leq 9$, $-25 \leq l \leq 25$ yielding 4555 unique reflections ($R_{int} = 0.0291$). The intensity data were corrected for Lorentz and polarization effects and for absorption using SADABSⁱⁱⁱ (minimum and maximum transmission 0.6464, 0.7452).

The structure was solved by direct methods (SHELXS-97^{iv}). Refinement was by full-matrix least squares based on F^2 using SHELXL-97.^v All reflections were used during refinement. The weighting scheme used was $w=1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.1950P]$ where $P = (F_o^2 + 2F_c^2)/3$. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using a riding model. Refinement converged to $R_1=0.0288$ and $wR_2=0.0776$ for 4423 observed reflections for which $F > 4\sigma(F)$ and $R_1=0.0299$ and $wR_2=0.0784$ and $GOF = 1.039$ for all 4555 unique, non-zero reflections and 305 variables.^{vi} The maximum Δ/σ in the final cycle of least squares was 0.011 and the two most prominent peaks in the final difference Fourier were +0.276 and -0.188 e/Å³.

Table 1 lists cell information, data collection parameters, and refinement data. Final positional and equivalent isotropic thermal parameters are given in **Tables 2** and **3**. Anisotropic thermal parameters are in **Table 4**. **Tables 5** and **6** list bond distances and bond angles. **Figure 1** is an ORTEP^{vii} representation of the molecule with 30% probability thermal ellipsoids displayed.

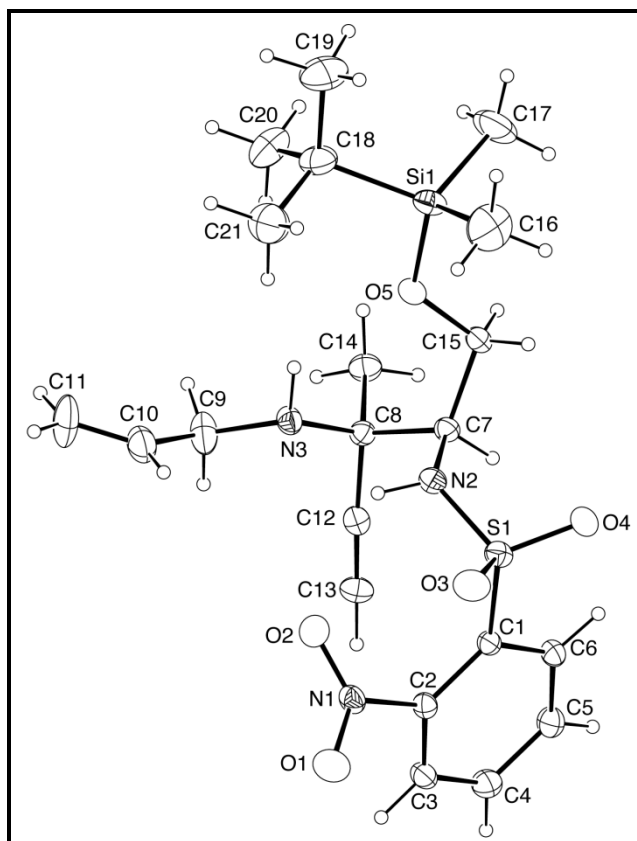


Figure 1. ORTEP drawing of the title compound with 30% probability thermal ellipsoids.

Table 1. Summary of Structure Determination of Compound 2a

Empirical formula	C ₂₁ H ₃₃ SiN ₃ SO ₅
Formula weight	467.65
Temperature	143(1) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P2 ₁
Cell constants:	
a	7.6795(2) Å
b	8.1287(2) Å
c	21.2564(5) Å
β	99.9650(10)°
Volume	1306.90(6) Å ³
Z	2
Density (calculated)	1.188 Mg/m ³
Absorption coefficient	0.203 mm ⁻¹
F(000)	500
Crystal size	0.38 x 0.30 x 0.12 mm ³
Theta range for data collection	1.95 to 25.05°
Index ranges	-9 ≤ h ≤ 9, -9 ≤ k ≤ 9, -25 ≤ l ≤ 25
Reflections collected	17678
Independent reflections	4555 [R(int) = 0.0291]
Completeness to theta = 25.05°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7452 and 0.6464
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4555 / 51 / 305
Goodness-of-fit on F ²	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0288, wR2 = 0.0776
R indices (all data)	R1 = 0.0299, wR2 = 0.0784
Absolute structure parameter	-0.02(5)
Largest diff. peak and hole	0.276 and -0.188 e.Å ⁻³

Table 2. Refined Positional Parameters for Compound 2a

Atom	x	y	z	$U_{eq}, \text{\AA}^2$
C1	0.6763(2)	0.6486(2)	0.43317(8)	0.0257(3)
C2	0.5297(2)	0.5746(2)	0.45167(8)	0.0268(3)
C3	0.5342(2)	0.5105(2)	0.51166(8)	0.0329(4)
C4	0.6910(3)	0.5139(3)	0.55519(9)	0.0385(4)
C5	0.8390(2)	0.5850(3)	0.53793(8)	0.0387(4)
C6	0.8310(2)	0.6553(2)	0.47789(8)	0.0316(4)
C7	0.8567(2)	0.5178(2)	0.30558(7)	0.0276(4)
C8	0.8108(2)	0.3315(2)	0.30298(8)	0.0272(3)
C9	0.5725(3)	0.1442(3)	0.25212(12)	0.0539(6)
C10	0.3836(7)	0.1606(7)	0.2161(2)	0.0519(11)
C11	0.2984(6)	0.0601(7)	0.1798(2)	0.0751(14)
C10'	0.4267(10)	0.1156(9)	0.1965(4)	0.059(2)
C11'	0.3154(10)	0.2301(14)	0.1788(4)	0.097(3)
C12	0.7718(2)	0.2857(2)	0.36637(8)	0.0288(4)
C13	0.7502(2)	0.2525(3)	0.41855(8)	0.0346(4)
C14	0.9683(2)	0.2285(3)	0.28973(9)	0.0378(4)
C15	0.9502(2)	0.5801(2)	0.25263(8)	0.0338(4)
C16	0.8138(5)	0.8403(3)	0.12147(16)	0.0806(9)
C17	1.1254(3)	0.6144(5)	0.11949(13)	0.0767(9)
C18	0.7478(3)	0.4948(3)	0.06084(9)	0.0506(5)
C19	0.7721(5)	0.5540(5)	-0.00575(11)	0.0853(10)
C20	0.8014(4)	0.3151(4)	0.06854(13)	0.0712(7)
C21	0.5529(3)	0.5104(5)	0.06593(12)	0.0717(8)
N1	0.36091(18)	0.5551(2)	0.40725(7)	0.0326(3)
N2	0.69075(17)	0.60948(19)	0.30531(6)	0.0291(3)
N3	0.64884(18)	0.30909(19)	0.25495(7)	0.0314(3)
O1	0.22591(16)	0.5851(2)	0.42858(7)	0.0545(4)
O2	0.36316(17)	0.50400(19)	0.35361(6)	0.0419(3)
O3	0.50574(18)	0.82352(18)	0.34099(7)	0.0426(3)
O4	0.83322(18)	0.84372(16)	0.36571(7)	0.0408(3)
O5	0.85313(16)	0.53738(18)	0.19158(6)	0.0370(3)
S1	0.67520(6)	0.74680(5)	0.357783(19)	0.03054(11)
Si1	0.88630(7)	0.62243(7)	0.12444(2)	0.03808(14)
$U_{eq} = \frac{1}{3}[U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha]$				

Table 3. Positional Parameters for Hydrogens in Compound 2a

Atom	x	y	z	$U_{\text{iso}}, \text{\AA}^2$
H3	0.4328	0.4652	0.5230	0.044
H4	0.6964	0.4686	0.5957	0.051
H5	0.9450	0.5859	0.5667	0.051
H6	0.9302	0.7073	0.4676	0.042
H7	0.9342	0.5393	0.3465	0.037
H9a	0.5729	0.1020	0.2948	0.072
H9b	0.6397	0.0697	0.2299	0.072
H9a'	0.5270	0.1243	0.2913	0.072
H9b'	0.6657	0.0647	0.2502	0.072
H10	0.3258	0.2582	0.2223	0.069
H11a	0.3492	-0.0398	0.1717	0.100
H11b	0.1831	0.0842	0.1604	0.100
H10'	0.4175	0.0153	0.1752	0.079
H11a'	0.3252	0.3302	0.2003	0.129
H11b'	0.2244	0.2135	0.1444	0.129
H13	0.7331	0.2264	0.4596	0.046
H14a	0.9437	0.1139	0.2946	0.057
H14b	1.0724	0.2585	0.3194	0.057
H14c	0.9873	0.2488	0.2469	0.057
H15a	0.9625	0.6988	0.2557	0.045
H15b	1.0676	0.5326	0.2577	0.045
H16a	0.6922	0.8458	0.1265	0.121
H16b	0.8265	0.8872	0.0811	0.121
H16c	0.8853	0.9006	0.1553	0.121
H17a	1.1921	0.6697	0.1557	0.115
H17b	1.1448	0.6675	0.0810	0.115
H17c	1.1627	0.5017	0.1192	0.115
H19a	0.6912	0.4964	-0.0378	0.128
H19b	0.8912	0.5325	-0.0116	0.128
H19c	0.7492	0.6700	-0.0095	0.128
H20a	0.7866	0.2774	0.1101	0.107
H20b	0.9230	0.3036	0.0640	0.107
H20c	0.7285	0.2508	0.0364	0.107
H21a	0.5153	0.6221	0.0576	0.108
H21b	0.5366	0.4798	0.1081	0.108
H21c	0.4841	0.4392	0.0352	0.108
H2a	0.5945	0.5490	0.2945	0.051
H3a	0.6722	0.3404	0.2164	0.051

Table 4. Refined Thermal Parameters (U's) for Compound 2a

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C1	0.0274(8)	0.0209(9)	0.0302(8)	-0.0020(6)	0.0089(6)	-0.0005(6)
C2	0.0215(7)	0.0255(8)	0.0337(8)	-0.0024(7)	0.0057(6)	0.0017(6)
C3	0.0297(9)	0.0314(10)	0.0400(10)	-0.0013(8)	0.0133(8)	-0.0035(7)
C4	0.0403(10)	0.0443(11)	0.0307(9)	0.0021(8)	0.0056(8)	-0.0026(8)
C5	0.0315(9)	0.0480(12)	0.0344(9)	-0.0022(8)	-0.0001(7)	-0.0064(8)
C6	0.0259(8)	0.0333(10)	0.0364(9)	-0.0048(7)	0.0084(7)	-0.0049(7)
C7	0.0227(7)	0.0328(9)	0.0276(8)	-0.0008(7)	0.0053(6)	-0.0003(7)
C8	0.0252(8)	0.0285(9)	0.0281(8)	-0.0011(7)	0.0052(6)	0.0014(7)
C9	0.0547(13)	0.0438(13)	0.0570(13)	0.0060(10)	-0.0080(10)	-0.0180(11)
C10	0.044(3)	0.057(3)	0.052(3)	0.000(2)	0.002(2)	-0.016(2)
C11	0.051(2)	0.064(3)	0.099(4)	-0.024(3)	-0.018(2)	-0.018(2)
C10'	0.049(4)	0.049(4)	0.078(5)	-0.043(4)	0.006(3)	-0.005(3)
C11'	0.054(4)	0.154(9)	0.080(5)	0.001(6)	0.000(4)	-0.013(5)
C12	0.0232(7)	0.0229(9)	0.0400(10)	0.0009(7)	0.0052(7)	0.0056(6)
C13	0.0359(9)	0.0359(9)	0.0340(9)	0.0073(8)	0.0121(7)	0.0091(8)
C14	0.0349(9)	0.0403(11)	0.0400(9)	-0.0017(9)	0.0112(7)	0.0080(8)
C15	0.0296(8)	0.0414(11)	0.0317(8)	-0.0003(7)	0.0087(7)	-0.0090(8)
C16	0.110(3)	0.0456(16)	0.085(2)	0.0120(14)	0.0151(17)	0.0095(17)
C17	0.0466(13)	0.115(3)	0.0762(17)	0.0025(18)	0.0327(12)	-0.0140(15)
C18	0.0543(13)	0.0654(15)	0.0329(10)	0.0015(10)	0.0096(9)	0.0035(11)
C19	0.106(2)	0.114(3)	0.0368(12)	0.0039(15)	0.0179(13)	-0.008(2)
C20	0.0912(19)	0.0629(16)	0.0578(15)	-0.0188(13)	0.0084(14)	0.0044(15)
C21	0.0519(14)	0.103(2)	0.0568(14)	0.0035(15)	-0.0011(11)	-0.0043(14)
N1	0.0214(7)	0.0372(8)	0.0392(8)	-0.0010(7)	0.0053(6)	-0.0017(6)
N2	0.0268(7)	0.0303(8)	0.0306(7)	0.0030(6)	0.0059(5)	0.0018(6)
N3	0.0287(7)	0.0337(8)	0.0304(7)	0.0031(6)	0.0017(6)	-0.0049(6)
O1	0.0217(6)	0.0837(13)	0.0590(9)	-0.0091(8)	0.0095(6)	0.0054(7)
O2	0.0289(6)	0.0546(9)	0.0398(7)	-0.0058(6)	-0.0004(5)	-0.0011(6)
O3	0.0477(8)	0.0342(7)	0.0480(8)	0.0097(6)	0.0142(6)	0.0148(6)
O4	0.0495(8)	0.0292(7)	0.0477(8)	-0.0012(6)	0.0196(6)	-0.0114(6)
O5	0.0352(6)	0.0468(8)	0.0300(6)	0.0015(6)	0.0088(5)	-0.0109(6)
S1	0.0354(2)	0.0235(2)	0.0347(2)	0.00327(17)	0.01159(17)	0.00174(17)
Si1	0.0413(3)	0.0408(3)	0.0358(3)	0.0068(2)	0.0170(2)	0.0017(2)
The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(a^2U_{11}h^2+b^2U_{22}k^2+c^2U_{33}l^2+2b*c*U_{23}kl+2a*c*U_{13}hl+2a*b*U_{12}hk)]$						

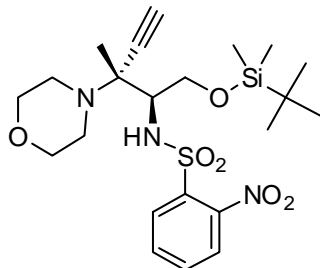
Table 5. Bond Distances in Compound 2a, Å

C1-C6	1.388(2)	C1-C2	1.392(2)	C1-S1	1.7888(16)
C2-C3	1.372(2)	C2-N1	1.474(2)	C3-C4	1.386(3)
C4-C5	1.380(3)	C5-C6	1.390(3)	C7-N2	1.476(2)
C7-C15	1.522(2)	C7-C8	1.554(2)	C8-N3	1.477(2)
C8-C12	1.478(2)	C8-C14	1.537(2)	C9-N3	1.460(3)
C9-C10'	1.499(8)	C9-C10	1.524(6)	C10-C11	1.232(6)
C10'-C11'	1.276(8)	C12-C13	1.181(2)	C15-O5	1.423(2)
C16-Si1	1.854(3)	C17-Si1	1.858(2)	C18-C20	1.519(4)
C18-C21	1.524(3)	C18-C19	1.537(3)	C18-Si1	1.881(2)
N1-O2	1.2166(19)	N1-O1	1.2257(19)	N2-S1	1.5970(15)
O3-S1	1.4314(14)	O4-S1	1.4321(14)	O5-Si1	1.6449(12)

Table 6. Bond Angles in Compound 2a, °

C6-C1-C2	117.48(15)	C6-C1-S1	117.85(12)	C2-C1-S1	124.55(12)
C3-C2-C1	122.35(15)	C3-C2-N1	115.61(14)	C1-C2-N1	122.01(15)
C2-C3-C4	119.47(16)	C5-C4-C3	119.41(17)	C4-C5-C6	120.58(16)
C1-C6-C5	120.62(16)	N2-C7-C15	110.27(14)	N2-C7-C8	107.53(13)
C15-C7-C8	115.54(14)	N3-C8-C12	108.65(13)	N3-C8-C14	113.65(14)
C12-C8-C14	108.65(14)	N3-C8-C7	107.68(13)	C12-C8-C7	107.11(13)
C14-C8-C7	110.88(15)	N3-C9-C10'	114.5(4)	N3-C9-C10	106.3(3)
C10'-C9-C10	26.0(2)	C11-C10-C9	127.9(6)	C11'-C10'-C9	119.4(7)
C13-C12-C8	176.11(18)	O5-C15-C7	110.70(13)	C20-C18-C21	108.9(2)
C20-C18-C19	109.0(2)	C21-C18-C19	108.5(2)	C20-C18-Si1	110.11(17)
C21-C18-Si1	110.08(17)	C19-C18-Si1	110.21(19)	O2-N1-O1	124.38(15)
O2-N1-C2	118.91(13)	O1-N1-C2	116.62(14)	C7-N2-S1	121.27(11)
C9-N3-C8	115.20(15)	C15-O5-Si1	123.59(11)	O3-S1-O4	120.33(9)
O3-S1-N2	107.75(8)	O4-S1-N2	107.60(8)	O3-S1-C1	106.33(8)
O4-S1-C1	105.50(8)	N2-S1-C1	108.93(7)	O5-Si1-C16	109.90(12)
O5-Si1-C17	109.70(11)	C16-Si1-C17	108.99(17)	O5-Si1-C18	103.80(9)
C16-Si1-C18	111.91(14)	C17-Si1-C18	112.43(13)		

X-ray Structure Determination of Compound 7a



Compound **7a**, C₂₂H₃₅SiN₃SO₆, crystallizes in the monoclinic space group C2 (systematic absences hkl: h+k=odd) with a=31.131(3)Å, b=7.8050(7)Å, c=22.844(2)Å, β=110.163(4)°, V=5210.5(8)Å³, Z=8, and d_{calc}=1.269 g/cm³. X-ray intensity data were collected on a Bruker APEXII CCD area detector employing graphite-monochromated Mo-Kα radiation (λ=0.71073 Å) at a temperature of 143(1)K. Preliminary indexing was performed from a series of thirty-six 0.5° rotation frames with exposures of 5 seconds. A total of 1581 frames were collected with a crystal to detector distance of 37.600 mm, rotation widths of 0.5° and exposures of 5 seconds:

scan type	2θ	ω	φ	χ	frames
φ	19.50	59.55	-7.81	-26.26	677
ω	-20.50	-25.09	-181.36	-31.86	169
φ	-10.50	300.13	-340.94	39.97	735

Rotation frames were integrated using SAINTⁱ, producing a listing of unaveraged F² and σ(F²) values which were then passed to the SHELXTLⁱⁱ program package for further processing and structure solution on a Dell Pentium 4 computer. A total of 35389 reflections were measured over the ranges 1.93 ≤ θ ≤ 25.05°, -36 ≤ h ≤ 36, -9 ≤ k ≤ 9, -26 ≤ l ≤ 27 yielding 9163 unique reflections (Rint = 0.0286). The intensity data were corrected for Lorentz and polarization effects and for absorption using SADABSⁱⁱⁱ (minimum and maximum transmission 0.6839, 0.7452).

The structure was solved by direct methods (SHELXS-97^{iv}). Refinement was by full-matrix least squares based on F² using SHELXL-97.^v All reflections were used during refinement. The weighting scheme used was w=1/[σ²(F_o²)+(0.0501P)²+0.2679P] where P = (F_o² + 2F_c²)/3. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using a riding model. Refinement converged to R1=0.0249 and wR2=0.0677 for 8717

observed reflections for which $F > 4\sigma(F)$ and $R1=0.0288$ and $wR2=0.0760$ and $GOF = 1.114$ for all 9163 unique, non-zero reflections and 608 variables.^{vi} The maximum Δ/σ in the final cycle of least squares was 0.005 and the two most prominent peaks in the final difference Fourier were +0.364 and -0.416 e/Å³.

Table 7 lists cell information, data collection parameters, and refinement data. Final positional and equivalent isotropic thermal parameters are given in **Tables 8** and **9**. Anisotropic thermal parameters are in **Table 10**. **Tables 11** and **12** list bond distances and bond angles. **Figures 2** and **3** are ORTEP^{vii} representations of the molecule with 30% probability thermal ellipsoids displayed.

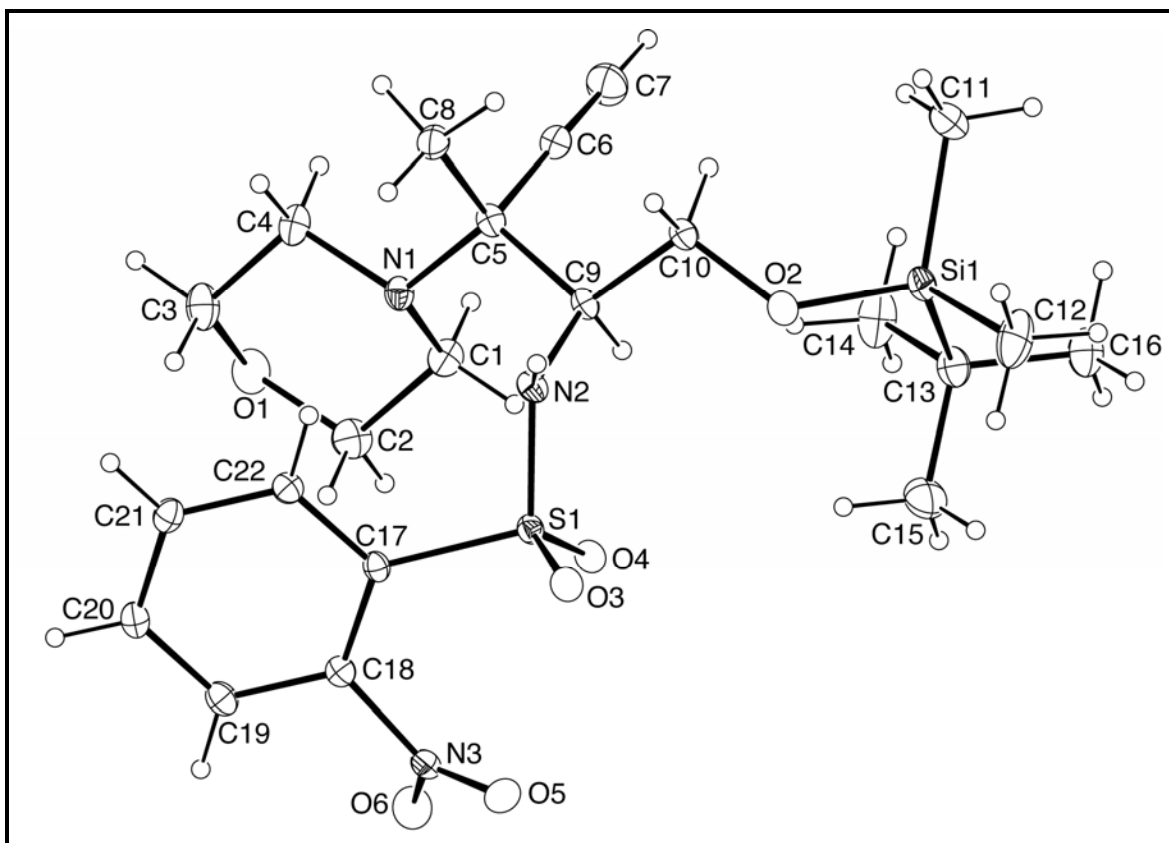


Figure 2. ORTEP drawing of molecule no. 1 of the asymmetric unit with 30% probability thermal ellipsoids.

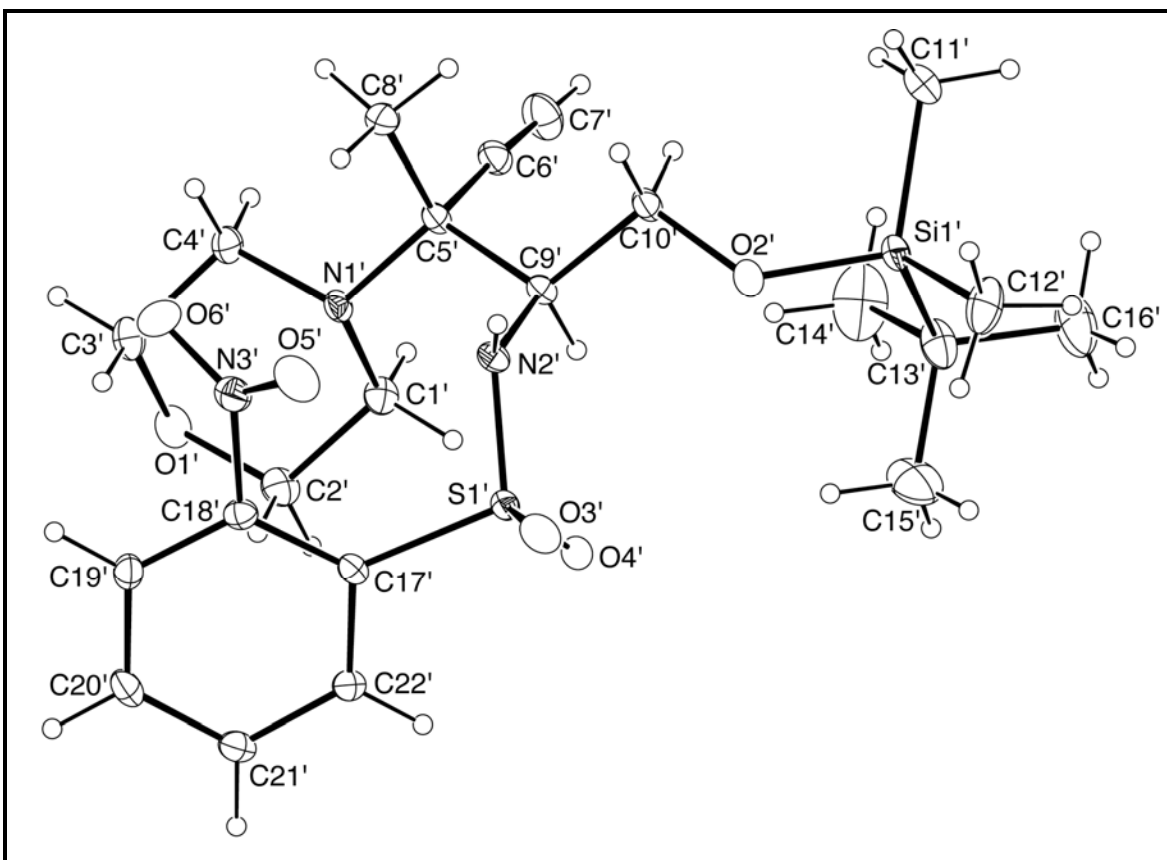


Figure 3. ORTEP drawing of molecule no. 2 of the asymmetric unit with 30% probability thermal ellipsoids.

Table 7. Summary of Structure Determination of Compound 7a

Empirical formula	C ₂₂ H ₃₅ SiN ₃ SO ₆
Formula weight	497.68
Temperature	143(1) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	C2
Cell constants:	
a	31.131(3) Å
b	7.8050(7) Å
c	22.844(2) Å
β	110.163(4)°
Volume	5210.5(8) Å ³
Z	8
Density (calculated)	1.269 Mg/m ³
Absorption coefficient	0.210 mm ⁻¹
F(000)	2128
Crystal size	0.44 x 0.20 x 0.18 mm ³
Theta range for data collection	1.93 to 25.05°
Index ranges	-36 ≤ h ≤ 36, -9 ≤ k ≤ 9, -26 ≤ l ≤ 27
Reflections collected	35389
Independent reflections	9163 [R(int) = 0.0286]
Completeness to theta = 25.05°	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7452 and 0.6839
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9163 / 1 / 608
Goodness-of-fit on F ²	1.114
Final R indices [I>2sigma(I)]	R1 = 0.0249, wR2 = 0.0677
R indices (all data)	R1 = 0.0288, wR2 = 0.0760
Absolute structure parameter	0.00(4)
Largest diff. peak and hole	0.364 and -0.416 e.Å ⁻³

Table 8. Refined Positional Parameters for Compound 7a

Atom	x	y	z	U _{eq} , Å ²
C1	0.65648(6)	0.5680(2)	0.26046(9)	0.0265(4)
C2	0.69972(6)	0.6415(3)	0.30573(9)	0.0319(4)
C3	0.72724(6)	0.3670(3)	0.33824(9)	0.0329(4)
C4	0.68344(6)	0.2883(2)	0.29453(8)	0.0278(4)
C5	0.59987(5)	0.3359(2)	0.24471(7)	0.0212(3)
C6	0.59693(6)	0.3251(2)	0.17801(8)	0.0259(4)
C7	0.59526(7)	0.3225(3)	0.12565(9)	0.0400(5)
C8	0.59264(6)	0.1575(2)	0.26765(8)	0.0269(4)
C9	0.56088(5)	0.4582(2)	0.24714(7)	0.0188(3)
C10	0.51344(5)	0.3933(2)	0.20623(8)	0.0217(4)
C11	0.43696(8)	0.4247(3)	0.06682(10)	0.0495(6)
C12	0.39159(6)	0.6465(3)	0.13811(12)	0.0475(6)
C13	0.47244(6)	0.7919(3)	0.10437(8)	0.0293(4)
C14	0.51743(7)	0.7462(3)	0.09455(11)	0.0454(6)
C15	0.48200(7)	0.9255(3)	0.15583(10)	0.0438(5)
C16	0.43902(7)	0.8659(3)	0.04318(9)	0.0395(5)
C17	0.62487(5)	0.6381(2)	0.40852(7)	0.0178(3)
C18	0.65218(5)	0.7750(2)	0.43823(7)	0.0192(3)
C19	0.69426(6)	0.7531(2)	0.48503(8)	0.0230(4)
C20	0.70928(5)	0.5894(2)	0.50439(7)	0.0233(4)
C21	0.68268(6)	0.4508(2)	0.47584(8)	0.0232(4)
C22	0.64117(5)	0.4743(2)	0.42781(8)	0.0205(4)
N1	0.64477(4)	0.40755(19)	0.28444(6)	0.0212(3)
N2	0.56067(4)	0.48331(18)	0.31066(6)	0.0194(3)
N3	0.63791(5)	0.95445(19)	0.42331(6)	0.0235(3)
O1	0.73708(4)	0.52566(18)	0.31500(6)	0.0328(3)
O2	0.48072(4)	0.52581(16)	0.19576(5)	0.0250(3)
O3	0.53723(4)	0.69314(17)	0.37458(5)	0.0253(3)
O4	0.57883(4)	0.79145(15)	0.30525(5)	0.0243(3)
O5	0.59946(4)	0.99629(17)	0.42071(6)	0.0328(3)
O6	0.66636(5)	1.05356(17)	0.41664(6)	0.0378(3)
S1	0.571152(12)	0.66542(5)	0.346154(18)	0.01795(9)
Si1	0.446531(15)	0.59539(6)	0.12717(2)	0.02413(11)
C1'	0.91217(6)	0.8394(2)	0.28112(8)	0.0247(4)
C2'	0.95354(5)	0.9082(3)	0.33196(9)	0.0287(4)
C3'	0.98077(6)	0.6323(3)	0.36054(8)	0.0289(4)
C4'	0.93920(5)	0.5569(2)	0.31059(8)	0.0259(4)
C5'	0.85694(5)	0.6003(2)	0.25106(7)	0.0197(3)
C6'	0.86065(6)	0.6025(2)	0.18743(8)	0.0254(4)
C7'	0.86402(6)	0.6138(3)	0.13782(9)	0.0376(5)
C8'	0.84821(6)	0.4171(2)	0.26833(8)	0.0259(4)
C9'	0.81538(5)	0.7168(2)	0.24769(7)	0.0180(3)
C10'	0.77037(5)	0.6524(2)	0.19951(8)	0.0225(4)

C11'	0.68742(8)	0.6611(3)	0.06596(10)	0.0505(6)
C12'	0.64643(6)	0.8991(3)	0.13804(11)	0.0440(5)
C13'	0.72337(6)	1.0324(3)	0.09368(9)	0.0369(5)
C14'	0.76809(8)	0.9837(4)	0.08401(14)	0.0718(9)
C15'	0.73280(10)	1.1769(3)	0.14177(11)	0.0623(7)
C16'	0.68900(8)	1.0961(4)	0.03177(11)	0.0563(7)
C17'	0.86456(5)	0.9149(2)	0.40877(7)	0.0189(3)
C18'	0.88748(6)	0.7760(2)	0.44374(8)	0.0209(4)
C19'	0.92874(6)	0.7953(2)	0.49248(8)	0.0235(4)
C20'	0.94670(6)	0.9559(2)	0.50856(8)	0.0254(4)
C21'	0.92439(6)	1.0965(2)	0.47530(8)	0.0251(4)
C22'	0.88392(6)	1.0753(2)	0.42516(8)	0.0224(4)
N1'	0.89935(4)	0.67092(18)	0.29814(6)	0.0193(3)
N2'	0.80977(4)	0.73011(18)	0.30864(6)	0.0188(3)
N3'	0.86915(5)	0.6015(2)	0.43338(7)	0.0285(3)
O1'	0.99210(4)	0.79733(17)	0.34376(6)	0.0286(3)
O2'	0.73652(4)	0.78027(16)	0.19062(5)	0.0254(3)
O3'	0.77582(4)	0.91350(19)	0.36931(6)	0.0333(3)
O4'	0.81562(4)	1.04629(16)	0.30403(5)	0.0301(3)
O5'	0.82928(5)	0.57992(19)	0.42992(6)	0.0399(3)
O6'	0.89551(5)	0.48693(17)	0.43115(7)	0.0427(4)
Si1'	0.811775(13)	0.90993(5)	0.343747(18)	0.02073(10)
Si1'	0.699468(15)	0.84194(6)	0.12264(2)	0.02436(11)
$U_{eq} = \frac{1}{3} [U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha]$				

Table 9. Positional Parameters for Hydrogens in Compound 7a

Atom	x	y	z	$U_{\text{iso}}, \text{\AA}^2$
H1a	0.6317	0.6495	0.2536	0.035
H1b	0.6605	0.5471	0.2208	0.035
H2a	0.7065	0.7496	0.2899	0.042
H2b	0.6956	0.6634	0.3453	0.042
H3a	0.7244	0.3853	0.3787	0.044
H3b	0.7524	0.2882	0.3436	0.044
H4a	0.6869	0.2622	0.2549	0.037
H4b	0.6772	0.1821	0.3122	0.037
H7	0.5939	0.3205	0.0844	0.053
H8a	0.6147	0.0795	0.2619	0.040
H8b	0.5623	0.1181	0.2443	0.040
H8c	0.5964	0.1631	0.3111	0.040
H9	0.5658	0.5700	0.2310	0.025
H10a	0.5146	0.3533	0.1666	0.029
H10b	0.5045	0.2977	0.2267	0.029
H11a	0.4648	0.4048	0.0587	0.074
H11b	0.4134	0.4605	0.0291	0.074
H11c	0.4277	0.3209	0.0816	0.074
H12a	0.3785	0.5434	0.1475	0.071
H12b	0.3709	0.6964	0.1006	0.071
H12c	0.3970	0.7262	0.1719	0.071
H14a	0.5307	0.8480	0.0844	0.068
H14b	0.5114	0.6652	0.0611	0.068
H14c	0.5383	0.6968	0.1321	0.068
H15a	0.4961	1.0241	0.1449	0.066
H15b	0.5022	0.8780	0.1942	0.066
H15c	0.4538	0.9587	0.1608	0.066
H16a	0.4105	0.8931	0.0485	0.059
H16b	0.4338	0.7828	0.0105	0.059
H16c	0.4518	0.9679	0.0324	0.059
H19	0.7121	0.8475	0.5031	0.031
H20	0.7371	0.5725	0.5364	0.031
H21	0.6927	0.3404	0.4890	0.031
H22	0.6241	0.3794	0.4084	0.027
H1a'	0.8868	0.9183	0.2740	0.033
H1b'	0.9187	0.8300	0.2427	0.033
H2a'	0.9611	1.0203	0.3200	0.038
H2b'	0.9465	0.9214	0.3699	0.038
H3a'	0.9747	0.6407	0.3993	0.038
H3b'	1.0067	0.5561	0.3674	0.038
H4a'	0.9459	0.5406	0.2725	0.034
H4b'	0.9322	0.4459	0.3241	0.034
H7'	0.8667	0.6228	0.0986	0.050

H8a'	0.8721	0.3432	0.2655	0.039
H8b'	0.8192	0.3779	0.2401	0.039
H8c'	0.8478	0.4154	0.3102	0.039
H9'	0.8214	0.8318	0.2352	0.024
H10a'	0.7748	0.6280	0.1603	0.030
H10b'	0.7608	0.5477	0.2143	0.030
H11a'	0.7147	0.6336	0.0572	0.076
H11b'	0.6636	0.6939	0.0280	0.076
H11c'	0.6777	0.5628	0.0834	0.076
H12a'	0.6329	0.7972	0.1476	0.066
H12b'	0.6252	0.9528	0.1018	0.066
H12c'	0.6538	0.9768	0.1727	0.066
H14a'	0.7622	0.8952	0.0531	0.108
H14b'	0.7897	0.9430	0.1226	0.108
H14c'	0.7804	1.0824	0.0703	0.108
H15a'	0.7528	1.1359	0.1814	0.094
H15b'	0.7045	1.2141	0.1456	0.094
H15c'	0.7470	1.2712	0.1285	0.094
H16a'	0.7005	1.1986	0.0192	0.084
H16b'	0.6603	1.1201	0.0370	0.084
H16c'	0.6847	1.0095	0.0004	0.084
H19'	0.9441	0.6998	0.5141	0.031
H20'	0.9739	0.9700	0.5419	0.034
H21'	0.9364	1.2057	0.4864	0.033
H22'	0.8696	1.1705	0.4022	0.030
H2	0.5402	0.4142	0.3219	0.030
H2'	0.7900	0.6618	0.3185	0.030

Table 10. Refined Thermal Parameters (U's) for Compound 7a

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C1	0.0225(8)	0.0256(10)	0.0334(10)	0.0034(8)	0.0122(7)	-0.0025(7)
C2	0.0221(9)	0.0342(11)	0.0413(10)	-0.0033(9)	0.0135(8)	-0.0060(8)
C3	0.0210(8)	0.0423(12)	0.0340(10)	0.0109(9)	0.0079(8)	-0.0010(8)
C4	0.0217(9)	0.0295(10)	0.0319(10)	0.0080(8)	0.0086(7)	0.0033(8)
C5	0.0191(8)	0.0237(9)	0.0192(8)	0.0014(7)	0.0047(7)	-0.0018(7)
C6	0.0234(8)	0.0252(9)	0.0269(10)	-0.0008(7)	0.0059(7)	0.0037(8)
C7	0.0449(12)	0.0497(13)	0.0268(11)	-0.0020(9)	0.0142(9)	0.0073(10)
C8	0.0235(8)	0.0211(9)	0.0322(9)	0.0011(8)	0.0044(7)	-0.0010(7)
C9	0.0161(7)	0.0224(8)	0.0164(7)	0.0005(7)	0.0038(6)	-0.0030(6)
C10	0.0173(8)	0.0240(9)	0.0208(8)	-0.0021(7)	0.0027(6)	-0.0015(7)
C11	0.0595(14)	0.0383(12)	0.0324(11)	-0.0090(10)	-0.0076(10)	0.0036(12)
C12	0.0205(9)	0.0552(14)	0.0664(15)	0.0211(12)	0.0143(9)	0.0066(10)
C13	0.0232(9)	0.0351(11)	0.0282(9)	0.0038(8)	0.0071(7)	-0.0007(8)
C14	0.0308(10)	0.0627(15)	0.0470(12)	0.0231(11)	0.0188(9)	0.0062(10)
C15	0.0462(12)	0.0309(11)	0.0443(12)	-0.0010(10)	0.0029(10)	-0.0109(10)
C16	0.0345(10)	0.0452(13)	0.0353(11)	0.0118(10)	0.0078(9)	0.0034(9)
C17	0.0170(7)	0.0225(9)	0.0140(7)	0.0014(6)	0.0054(6)	0.0004(7)
C18	0.0200(8)	0.0205(9)	0.0178(8)	0.0012(7)	0.0076(7)	-0.0011(7)
C19	0.0197(8)	0.0272(9)	0.0213(8)	-0.0012(7)	0.0061(7)	-0.0040(7)
C20	0.0191(8)	0.0292(10)	0.0201(8)	0.0025(7)	0.0047(7)	0.0018(7)
C21	0.0242(8)	0.0235(9)	0.0227(8)	0.0043(7)	0.0091(7)	0.0041(7)
C22	0.0198(8)	0.0210(9)	0.0211(8)	0.0000(7)	0.0073(7)	-0.0019(7)
N1	0.0152(6)	0.0239(7)	0.0235(7)	0.0023(6)	0.0053(5)	-0.0016(6)
N2	0.0180(7)	0.0220(7)	0.0182(7)	0.0003(6)	0.0060(5)	-0.0056(6)
N3	0.0261(8)	0.0213(8)	0.0182(7)	-0.0025(6)	0.0016(6)	-0.0006(6)
O1	0.0183(6)	0.0402(8)	0.0417(8)	0.0039(6)	0.0125(5)	-0.0046(6)
O2	0.0206(6)	0.0309(7)	0.0219(6)	-0.0018(5)	0.0053(5)	0.0026(5)
O3	0.0189(5)	0.0307(7)	0.0259(6)	-0.0027(5)	0.0072(5)	0.0008(5)
O4	0.0268(6)	0.0213(6)	0.0210(6)	0.0019(5)	0.0033(5)	-0.0025(5)
O5	0.0305(7)	0.0291(7)	0.0363(7)	-0.0049(6)	0.0082(6)	0.0070(6)
O6	0.0354(7)	0.0261(7)	0.0448(8)	0.0066(6)	0.0047(6)	-0.0096(6)
S1	0.01546(18)	0.0188(2)	0.01773(19)	0.00040(15)	0.00339(15)	-0.00106(16)
Si1	0.0174(2)	0.0275(3)	0.0232(2)	-0.0009(2)	0.00142(19)	-0.00089(19)
C1'	0.0198(8)	0.0257(9)	0.0283(9)	0.0032(8)	0.0080(7)	-0.0034(7)
C2'	0.0186(8)	0.0313(10)	0.0359(10)	-0.0030(8)	0.0089(7)	-0.0066(8)
C3'	0.0175(8)	0.0374(11)	0.0291(9)	0.0028(8)	0.0044(7)	0.0000(8)
C4'	0.0170(8)	0.0282(10)	0.0294(9)	0.0001(8)	0.0039(7)	0.0017(7)
C5'	0.0164(8)	0.0237(8)	0.0169(8)	-0.0026(7)	0.0032(6)	-0.0017(7)
C6'	0.0193(8)	0.0301(10)	0.0249(9)	-0.0068(8)	0.0052(7)	0.0008(7)
C7'	0.0348(10)	0.0552(14)	0.0234(10)	-0.0034(9)	0.0108(8)	0.0030(10)
C8'	0.0227(8)	0.0217(9)	0.0299(9)	-0.0035(8)	0.0047(7)	-0.0011(8)
C9'	0.0163(7)	0.0205(8)	0.0168(7)	-0.0023(7)	0.0051(6)	-0.0025(7)
C10'	0.0166(8)	0.0287(10)	0.0193(8)	-0.0045(7)	0.0025(6)	0.0006(7)

C11'	0.0506(13)	0.0435(13)	0.0354(11)	-0.0119(10)	-0.0135(10)	0.0052(11)
C12'	0.0238(9)	0.0524(14)	0.0563(13)	0.0181(12)	0.0144(9)	0.0099(10)
C13'	0.0298(10)	0.0462(12)	0.0299(10)	0.0104(9)	0.0044(8)	-0.0068(9)
C14'	0.0465(14)	0.098(2)	0.0804(19)	0.0341(18)	0.0346(14)	-0.0011(15)
C15'	0.0837(18)	0.0375(13)	0.0512(14)	0.0034(11)	0.0047(13)	-0.0267(14)
C16'	0.0517(13)	0.0662(17)	0.0397(12)	0.0241(12)	0.0014(11)	-0.0117(13)
C17'	0.0175(7)	0.0227(8)	0.0161(7)	-0.0024(7)	0.0054(6)	-0.0016(7)
C18'	0.0246(9)	0.0200(9)	0.0197(8)	-0.0010(7)	0.0099(7)	-0.0002(7)
C19'	0.0232(8)	0.0269(9)	0.0191(8)	0.0020(7)	0.0054(7)	0.0055(7)
C20'	0.0172(8)	0.0375(11)	0.0196(8)	-0.0061(8)	0.0039(7)	-0.0007(7)
C21'	0.0248(9)	0.0241(9)	0.0261(9)	-0.0064(8)	0.0083(7)	-0.0038(8)
C22'	0.0246(8)	0.0200(9)	0.0221(9)	-0.0014(7)	0.0074(7)	0.0002(7)
N1'	0.0132(6)	0.0228(7)	0.0198(7)	-0.0013(6)	0.0029(5)	-0.0014(6)
N2'	0.0170(6)	0.0212(7)	0.0183(7)	-0.0023(6)	0.0064(5)	-0.0045(6)
N3'	0.0390(9)	0.0231(8)	0.0200(7)	0.0028(6)	0.0056(7)	-0.0044(7)
O1'	0.0156(6)	0.0363(8)	0.0338(7)	0.0009(6)	0.0082(5)	-0.0042(5)
O2'	0.0190(6)	0.0341(7)	0.0209(6)	-0.0029(5)	0.0039(5)	0.0054(5)
O3'	0.0199(6)	0.0465(8)	0.0335(7)	-0.0140(6)	0.0093(5)	0.0005(6)
O4'	0.0361(7)	0.0217(6)	0.0227(6)	0.0008(5)	-0.0025(5)	0.0019(6)
O5'	0.0407(8)	0.0400(9)	0.0348(7)	0.0048(7)	0.0076(6)	-0.0191(7)
O6'	0.0609(10)	0.0206(7)	0.0401(8)	0.0021(6)	0.0091(7)	0.0053(7)
S1'	0.01686(19)	0.0223(2)	0.01968(19)	-0.00398(17)	0.00198(15)	0.00162(17)
Si1'	0.0167(2)	0.0286(3)	0.0230(2)	-0.0011(2)	0.00063(18)	0.00033(19)
The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$						

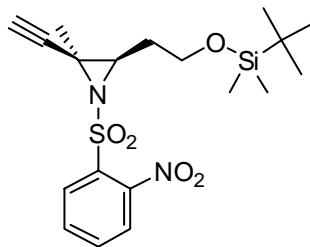
Table 11. Bond Distances in Compound 7a, Å

C1-N1	1.463(2)	C1-C2	1.500(2)	C2-O1	1.430(2)
C3-O1	1.422(2)	C3-C4	1.515(2)	C4-N1	1.476(2)
C5-N1	1.488(2)	C5-C6	1.497(2)	C5-C8	1.531(2)
C5-C9	1.560(2)	C6-C7	1.179(3)	C9-N2	1.466(2)
C9-C10	1.536(2)	C10-O2	1.413(2)	C11-Si1	1.866(2)
C12-Si1	1.855(2)	C13-C15	1.522(3)	C13-C14	1.535(3)
C13-C16	1.538(3)	C13-Si1	1.888(2)	C17-C18	1.388(2)
C17-C22	1.390(2)	C17-S1	1.7972(16)	C18-C19	1.387(2)
C18-N3	1.474(2)	C19-C20	1.380(3)	C20-C21	1.382(3)
C21-C22	1.389(2)	N2-S1	1.6130(14)	N3-O5	1.2223(19)
N3-O6	1.224(2)	O2-Si1	1.6532(12)	O3-S1	1.4340(12)
O4-S1	1.4324(12)	C1'-N1'	1.465(2)	C1'-C2'	1.505(2)
C2'-O1'	1.428(2)	C3'-O1'	1.423(2)	C3'-C4'	1.518(2)
C4'-N1'	1.473(2)	C5'-N1'	1.4915(19)	C5'-C6'	1.497(2)
C5'-C8'	1.532(2)	C5'-C9'	1.562(2)	C6'-C7'	1.177(3)
C9'-N2'	1.465(2)	C9'-C10'	1.538(2)	C10'-O2'	1.414(2)
C11'-Si1'	1.864(2)	C12'-Si1'	1.857(2)	C13'-C15'	1.530(3)
C13'-C14'	1.531(3)	C13'-C16'	1.533(3)	C13'-Si1'	1.882(2)
C17'-C22'	1.383(2)	C17'-C18'	1.389(2)	C17'-S1'	1.7960(15)
C18'-C19'	1.388(2)	C18'-N3'	1.464(2)	C19'-C20'	1.370(3)
C20'-C21'	1.379(3)	C21'-C22'	1.390(2)	N2'-S1'	1.6071(14)
N3'-O6'	1.227(2)	N3'-O5'	1.228(2)	O2'-Si1'	1.6550(12)
O3'-S1'	1.4301(12)	O4'-S1'	1.4302(13)		

Table 12. Bond Angles in Compound 7a, °

N1-C1-C2	110.47(15)	O1-C2-C1	110.54(16)	O1-C3-C4	111.59(15)
N1-C4-C3	110.35(16)	N1-C5-C6	110.91(13)	N1-C5-C8	110.55(13)
C6-C5-C8	109.44(15)	N1-C5-C9	109.08(13)	C6-C5-C9	107.17(13)
C8-C5-C9	109.64(13)	C7-C6-C5	177.6(2)	N2-C9-C10	108.35(12)
N2-C9-C5	112.71(13)	C10-C9-C5	111.93(13)	O2-C10-C9	110.34(14)
C15-C13-C14	109.07(17)	C15-C13-C16	109.62(17)	C14-C13-C16	108.65(15)
C15-C13-Si1	109.38(13)	C14-C13-Si1	110.46(14)	C16-C13-Si1	109.64(13)
C18-C17-C22	117.25(14)	C18-C17-S1	122.83(13)	C22-C17-S1	119.90(12)
C19-C18-C17	122.61(15)	C19-C18-N3	115.13(15)	C17-C18-N3	122.24(14)
C20-C19-C18	119.13(16)	C19-C20-C21	119.48(15)	C20-C21-C22	120.82(16)
C21-C22-C17	120.67(16)	C1-N1-C4	107.65(13)	C1-N1-C5	113.35(13)
C4-N1-C5	113.72(14)	C9-N2-S1	123.11(11)	O5-N3-O6	124.29(15)
O5-N3-C18	118.51(15)	O6-N3-C18	117.14(14)	C3-O1-C2	109.70(13)
C10-O2-Si1	126.29(10)	O4-S1-O3	120.42(8)	O4-S1-N2	109.12(7)
O3-S1-N2	107.91(7)	O4-S1-C17	106.24(7)	O3-S1-C17	106.75(7)
N2-S1-C17	105.41(7)	O2-Si1-C12	105.38(9)	O2-Si1-C11	110.63(8)
C12-Si1-C11	109.46(12)	O2-Si1-C13	109.37(7)	C12-Si1-C13	111.33(10)
C11-Si1-C13	110.55(11)	N1'-C1'-C2'	110.74(14)	O1'-C2'-C1'	111.71(15)
O1'-C3'-C4'	111.99(15)	N1'-C4'-C3'	110.75(15)	N1'-C5'-C6'	110.51(13)
N1'-C5'-C8'	110.54(13)	C6'-C5'-C8'	109.91(14)	N1'-C5'-C9'	109.44(13)
C6'-C5'-C9'	106.58(13)	C8'-C5'-C9'	109.78(13)	C7'-C6'-C5'	176.3(2)
N2'-C9'-C10'	109.01(12)	N2'-C9'-C5'	111.25(13)	C10'-C9'-C5'	112.35(13)
O2'-C10'-C9'	108.79(14)	C15'-C13'-C14'	109.1(2)	C15'-C13'-C16'	108.9(2)
C14'-C13'-C16'	109.15(19)	C15'-C13'-Si1'	109.31(14)	C14'-C13'-Si1'	110.12(17)
C16'-C13'-Si1'	110.22(15)	C22'-C17'-C18'	117.45(14)	C22'-C17'-S1'	115.63(13)
C18'-C17'-S1'	126.92(13)	C19'-C18'-C17'	121.76(16)	C19'-C18'-N3'	115.61(15)
C17'-C18'-N3'	122.60(15)	C20'-C19'-C18'	119.59(16)	C19'-C20'-C21'	119.94(15)
C20'-C21'-C22'	120.02(16)	C17'-C22'-C21'	121.18(16)	C1'-N1'-C4'	107.77(13)
C1'-N1'-C5'	113.25(12)	C4'-N1'-C5'	113.16(13)	C9'-N2'-S1'	122.65(11)
O6'-N3'-O5'	124.98(16)	O6'-N3'-C18'	117.11(15)	O5'-N3'-C18'	117.85(15)
C3'-O1'-C2'	109.22(12)	C10'-O2'-Si1'	125.72(10)	O3'-S1'-O4'	119.55(8)
O3'-S1'-N2'	108.64(8)	O4'-S1'-N2'	109.30(7)	O3'-S1'-C17'	106.48(7)
O4'-S1'-C17'	104.82(8)	N2'-S1'-C17'	107.39(8)	O2'-Si1'-C12'	105.65(8)
O2'-Si1'-C11'	109.87(8)	C12'-Si1'-C11'	109.52(11)	O2'-Si1'-C13'	109.11(8)
C12'-Si1'-C13'	111.23(10)	C11'-Si1'-C13'	111.30(11)		

X-ray Structure Determination of Compound 20



Compound **20**, C₁₉H₂₈SiN₂SO₅, crystallizes in the monoclinic space group P2₁ (systematic absences 0k0: k=odd) with a=7.2155(4)Å, b=7.3686(4)Å, c=21.8244(11)Å, β=91.207(3)°, V=1160.11(11)Å³, Z=2, and d_{calc}=1.215 g/cm³. X-ray intensity data were collected on a Bruker APEXII CCD area detector employing graphite-monochromated Mo-Kα radiation (λ=0.71073 Å) at a temperature of 158(1)K. Preliminary indexing was performed from a series of thirty-six 0.5° rotation frames with exposures of 30 seconds. A total of 2839 frames were collected with a crystal to detector distance of 37.508 mm, rotation widths of 0.5° and exposures of 30 seconds:

scan type	2θ	ω	φ	χ	frames
φ	-15.50	258.48	-351.72	19.46	732
ω	-20.50	-26.83	-181.36	-31.86	204
ω	9.50	-40.83	-60.64	88.14	104
ω	4.50	-53.38	-128.06	52.47	109
φ	22.00	14.84	73.18	97.50	404
φ	-10.50	300.13	23.20	39.97	565
φ	19.50	59.55	-9.72	-26.26	721

Rotation frames were integrated using SAINTⁱ, producing a listing of unaveraged F² and α(F²) values which were then passed to the SHELXTLⁱⁱ program package for further processing and structure solution on a Dell Pentium 4 computer. A total of 27690 reflections were measured over the ranges 1.87 ≤ θ ≤ 25.22°, -8 ≤ h ≤ 8, -8 ≤ k ≤ 8, -26 ≤ l ≤ 26 yielding 4153 unique reflections (Rint = 0.0420). The intensity data were corrected for Lorentz and polarization effects and for absorption using SADABSⁱⁱⁱ (minimum and maximum transmission 0.6269, 0.7452).

The structure was solved by direct methods (SHELXS-97^{iv}). The -OTBS substituent is disordered by a slight rotation around the C12-C13 Bond; the two contributing disorder models (O5, Si1, C14-C18 and O5', Si1', C14'-C18') had relative occupancies of 60% and 40%. Refinement was by full-matrix least squares based on F² using SHELXL-97.^v All reflections were used during refinement. The weighting scheme used was w=1/[α²(F_o²) + (0.0550P)² + 0.3223P] where P = (F_o² + 2F_c²)/3. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using a riding model. Refinement converged to R1=0.0432 and wR2=0.1026 for 3445 observed reflections for which F > 4σ(F) and R1=0.0580 and wR2=0.1108 and GOF =1.036 for all 4153 unique, non-zero reflections and 327 variables.^{vi} The maximum Δ/σ in the final cycle of least squares was 0.036 and the two most prominent peaks in

the final difference Fourier were +0.387 and -0.199 e/Å³.

Table 13 lists cell information, data collection parameters, and refinement data. Final positional and equivalent isotropic thermal parameters are given in **Tables 14** and **15**. Anisotropic thermal parameters are in **Table 16**. **Tables 17** and **18** list bond distances and bond angles. **Figure 4** is an ORTEP^{vii} representation of the molecule with 30% probability thermal ellipsoids displayed.

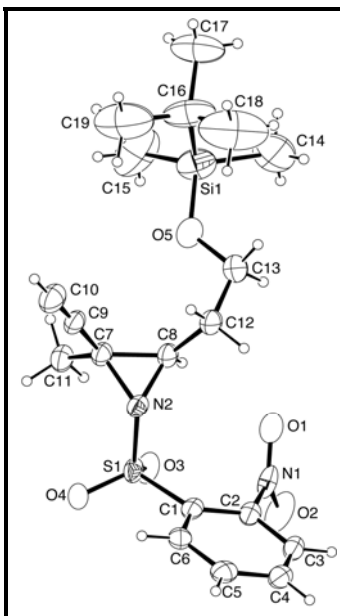


Figure 4. ORTEP drawing of the title compound with 30% probability thermal ellipsoids.

Table 13. Summary of Structure Determination of Compound 20

Empirical formula	C ₁₉ H ₂₈ SiN ₂ SO ₅
Formula weight	424.58
Temperature	158(1) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P2 ₁
Cell constants:	
a	7.2155(4) Å
b	7.3686(4) Å
c	21.8244(11) Å
β	91.207(3)°
Volume	1160.11(11) Å ³
Z	2
Density (calculated)	1.215 Mg/m ³
Absorption coefficient	0.221 mm ⁻¹
F(000)	452
Crystal size	0.38 x 0.18 x 0.05 mm ³
Theta range for data collection	1.87 to 25.22°
Index ranges	-8 ≤ h ≤ 8, -8 ≤ k ≤ 8, -26 ≤ l ≤ 26
Reflections collected	27690
Independent reflections	4153 [R(int) = 0.0420]
Completeness to theta = 25.22°	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7452 and 0.6269
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4153 / 83 / 327
Goodness-of-fit on F ²	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0432, wR2 = 0.1026
R indices (all data)	R1 = 0.0580, wR2 = 0.1108
Absolute structure parameter	0.01(9)
Largest diff. peak and hole	0.387 and -0.199 e.Å ⁻³

Table 14. Refined Positional Parameters for Compound 20

Atom	x	y	z	U _{eq} , Å ²
C1	0.7630(4)	0.5916(4)	0.55895(14)	0.0437(7)
C2	0.8259(3)	0.4127(4)	0.56240(14)	0.0445(7)
C3	0.8184(4)	0.2985(4)	0.51241(15)	0.0506(8)
C4	0.7420(4)	0.3612(5)	0.45854(16)	0.0551(8)
C5	0.6748(4)	0.5366(5)	0.45390(15)	0.0535(8)
C6	0.6872(4)	0.6523(4)	0.50379(14)	0.0494(7)
C7	0.5476(4)	0.8188(4)	0.71216(14)	0.0457(7)
C8	0.5583(4)	0.6198(4)	0.70669(14)	0.0467(7)
C9	0.3675(5)	0.9079(4)	0.71104(14)	0.0509(7)
C10	0.2276(6)	0.9805(5)	0.70917(17)	0.0731(10)
C11	0.6960(4)	0.9226(4)	0.74720(15)	0.0568(8)
C12	0.3965(5)	0.4940(5)	0.70473(15)	0.0618(9)
C13	0.3762(7)	0.3982(6)	0.7655(2)	0.0924(14)
N1	0.9025(4)	0.3361(4)	0.61993(16)	0.0620(8)
N2	0.5855(3)	0.7302(3)	0.65157(10)	0.0426(5)
O1	0.7961(4)	0.3131(3)	0.66196(13)	0.0748(7)
O2	1.0652(4)	0.2941(4)	0.62035(14)	0.0929(10)
O3	0.9387(3)	0.6859(3)	0.65832(11)	0.0598(6)
O4	0.7972(3)	0.9259(3)	0.59424(11)	0.0609(6)
S1	0.78948(9)	0.74787(9)	0.61995(4)	0.0465(2)
O5	0.3833(11)	0.5184(14)	0.8176(3)	0.077(2)
Si1	0.3052(5)	0.4755(5)	0.88561(11)	0.0974(9)
C14	0.357(3)	0.2303(14)	0.9051(8)	0.153(6)
C15	0.4292(18)	0.6361(18)	0.9371(6)	0.170(5)
C16	0.0434(10)	0.5063(16)	0.8867(3)	0.134(3)
C17	-0.0331(15)	0.4590(19)	0.9496(4)	0.159(5)
C18	-0.053(2)	0.392(3)	0.8372(6)	0.227(10)
C19	0.007(2)	0.7093(17)	0.8744(6)	0.205(7)
O5'	0.3116(15)	0.547(2)	0.8038(4)	0.068(3)
Si1'	0.2096(6)	0.4897(6)	0.86718(16)	0.0853(11)
C14'	0.354(3)	0.319(3)	0.9101(12)	0.139(7)
C15'	-0.0307(17)	0.418(3)	0.8477(10)	0.133(7)
C16'	0.1988(15)	0.7044(13)	0.9126(4)	0.110(3)
C17'	0.3926(16)	0.779(2)	0.9198(7)	0.136(6)
C18'	0.070(2)	0.836(2)	0.8790(6)	0.125(5)
C19'	0.119(2)	0.654(2)	0.9753(5)	0.169(7)
$U_{eq} = \frac{1}{3}[U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha]$				

Table 15. Positional Parameters for Hydrogens in Compound 20

Atom	x	y	z	U _{iso} , Å ²
H3	0.8646	0.1808	0.5152	0.067
H4	0.7350	0.2849	0.4246	0.073
H5	0.6214	0.5769	0.4172	0.071
H6	0.6444	0.7710	0.5003	0.066
H8	0.6723	0.5665	0.7240	0.062
H10	0.1137	1.0396	0.7076	0.097
H11a	0.7180	1.0363	0.7271	0.085
H11b	0.8083	0.8528	0.7485	0.085
H11c	0.6559	0.9447	0.7882	0.085
H12a	0.4131	0.4048	0.6726	0.082
H12b	0.2845	0.5620	0.6952	0.082
H13a	0.2588	0.3338	0.7652	0.123
H13b	0.4742	0.3088	0.7701	0.123
H14a	0.2889	0.1524	0.8776	0.229
H14b	0.3214	0.2061	0.9465	0.229
H14c	0.4874	0.2081	0.9013	0.229
H15a	0.3939	0.7581	0.9268	0.255
H15b	0.5605	0.6221	0.9325	0.255
H15c	0.3976	0.6115	0.9788	0.255
H17a	0.0242	0.5352	0.9803	0.239
H17b	-0.0066	0.3341	0.9589	0.239
H17c	-0.1647	0.4779	0.9492	0.239
H18a	-0.0049	0.4237	0.7979	0.340
H18b	-0.1837	0.4155	0.8374	0.340
H18c	-0.0305	0.2660	0.8452	0.340
H19a	0.0642	0.7802	0.9066	0.308
H19b	-0.1238	0.7315	0.8732	0.308
H19c	0.0592	0.7426	0.8359	0.308
H14a'	0.4759	0.3682	0.9178	0.208
H14b'	0.3640	0.2105	0.8861	0.208
H14c'	0.2974	0.2915	0.9484	0.208
H15a'	-0.0902	0.5102	0.8231	0.200
H15b'	-0.0983	0.4014	0.8847	0.200
H15c'	-0.0281	0.3064	0.8252	0.200
H17a'	0.4696	0.6919	0.9409	0.204
H17b'	0.3897	0.8896	0.9430	0.204
H17c'	0.4421	0.8028	0.8801	0.204
H18a'	-0.0510	0.7836	0.8750	0.188
H18b'	0.1176	0.8603	0.8390	0.188
H18c'	0.0636	0.9472	0.9017	0.188
H19a'	0.2009	0.5692	0.9957	0.253
H19b'	-0.0006	0.5988	0.9693	0.253
H19c'	0.1076	0.7609	0.9998	0.253

Table 16. Refined Thermal Parameters (U's) for Compound 20

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C1	0.0280(14)	0.0459(16)	0.0576(18)	-0.0118(14)	0.0090(13)	-0.0049(12)
C2	0.0258(13)	0.0439(16)	0.0638(18)	-0.0116(15)	0.0037(12)	-0.0043(12)
C3	0.0337(14)	0.0427(18)	0.076(2)	-0.0173(15)	0.0116(14)	-0.0080(11)
C4	0.0430(17)	0.058(2)	0.064(2)	-0.0202(16)	0.0118(15)	-0.0154(15)
C5	0.0374(16)	0.067(2)	0.0569(18)	-0.0060(16)	0.0083(15)	-0.0091(14)
C6	0.0374(15)	0.0474(17)	0.064(2)	-0.0010(15)	0.0146(14)	-0.0018(12)
C7	0.0516(17)	0.0408(15)	0.0449(17)	-0.0070(13)	-0.0002(14)	-0.0012(13)
C8	0.0509(18)	0.0394(16)	0.0496(18)	-0.0097(13)	0.0006(14)	-0.0055(13)
C9	0.0536(19)	0.0433(16)	0.0561(18)	-0.0174(15)	0.0093(15)	-0.0035(15)
C10	0.062(2)	0.069(2)	0.088(3)	-0.026(2)	0.008(2)	-0.0075(19)
C11	0.0587(19)	0.0468(17)	0.065(2)	-0.0101(16)	-0.0002(15)	-0.0011(15)
C12	0.069(2)	0.0493(19)	0.067(2)	-0.0193(17)	0.0159(17)	-0.0160(16)
C13	0.125(4)	0.059(2)	0.096(3)	-0.019(2)	0.043(3)	-0.027(2)
N1	0.0639(19)	0.0397(14)	0.082(2)	-0.0218(14)	-0.0152(17)	0.0160(14)
N2	0.0371(11)	0.0426(13)	0.0480(12)	-0.0114(12)	0.0018(9)	-0.0007(11)
O1	0.109(2)	0.0479(14)	0.0676(17)	-0.0044(11)	0.0024(16)	0.0099(13)
O2	0.0670(16)	0.083(2)	0.127(2)	-0.0373(17)	-0.0328(15)	0.0395(14)
O3	0.0372(11)	0.0509(12)	0.0909(16)	-0.0222(11)	-0.0116(10)	0.0012(8)
O4	0.0648(14)	0.0365(12)	0.0820(15)	-0.0095(11)	0.0185(12)	-0.0079(10)
S1	0.0352(3)	0.0368(3)	0.0676(5)	-0.0133(4)	0.0038(3)	-0.0036(3)
O5	0.108(6)	0.063(4)	0.060(3)	-0.010(3)	0.001(3)	0.004(4)
Si1	0.110(2)	0.136(2)	0.0449(13)	0.0052(13)	-0.0152(12)	0.0106(18)
C14	0.220(14)	0.146(9)	0.092(8)	0.052(8)	0.008(8)	0.029(10)
C15	0.209(11)	0.201(12)	0.097(7)	-0.066(9)	-0.055(8)	0.034(10)
C16	0.114(6)	0.239(11)	0.050(4)	0.020(6)	0.011(4)	0.035(7)
C17	0.141(8)	0.244(15)	0.094(5)	0.049(8)	0.040(6)	0.013(9)
C18	0.125(11)	0.44(3)	0.117(9)	-0.008(15)	-0.022(9)	-0.084(16)
C19	0.189(14)	0.280(13)	0.149(12)	0.102(11)	0.051(9)	0.121(12)
O5'	0.093(7)	0.063(6)	0.049(5)	0.002(4)	0.019(5)	-0.013(6)
Si1'	0.097(3)	0.110(3)	0.049(2)	0.0125(18)	0.0134(18)	-0.028(2)
C14'	0.178(15)	0.124(11)	0.112(14)	0.062(12)	-0.020(12)	-0.017(11)
C15'	0.086(8)	0.190(18)	0.126(16)	-0.013(13)	0.037(9)	-0.028(10)
C16'	0.125(8)	0.153(9)	0.053(5)	-0.006(5)	0.021(5)	0.004(7)
C17'	0.158(10)	0.154(16)	0.095(11)	-0.048(11)	-0.011(8)	-0.021(10)
C18'	0.156(12)	0.152(11)	0.069(8)	-0.018(8)	0.018(8)	0.041(11)
C19'	0.31(2)	0.141(14)	0.060(7)	-0.007(7)	0.066(10)	-0.027(14)

The form of the anisotropic displacement parameter is:

$$\exp[-2\pi^2(a^2U_{11}h^2+b^2U_{22}k^2+c^2U_{33}l^2+2b*c*U_{23}kl+2a*c*U_{13}hl+2a*b*U_{12}hk)]$$

Table 17. Bond Distances in Compound 20, Å

C1-C6	1.386(4)	C1-C2	1.396(4)	C1-S1	1.767(3)
C2-C3	1.378(4)	C2-N1	1.473(4)	C3-C4	1.369(5)
C4-C5	1.384(5)	C5-C6	1.384(4)	C7-C9	1.455(5)
C7-C8	1.474(4)	C7-N2	1.505(4)	C7-C11	1.511(4)
C8-N2	1.469(4)	C8-C12	1.490(4)	C9-C10	1.143(5)
C12-C13	1.513(5)	C13-O5	1.441(10)	C13-O5'	1.464(14)
N1-O2	1.214(3)	N1-O1	1.221(4)	N2-S1	1.644(2)
O3-S1	1.425(2)	O4-S1	1.429(2)	O5-Si1	1.630(6)
Si1-C15	1.851(8)	Si1-C14	1.892(8)	Si1-C16	1.903(7)
C16-C18	1.524(8)	C16-C17	1.531(7)	C16-C19	1.541(9)
O5'-Si1'	1.636(7)	Si1'-C15'	1.853(10)	Si1'-C14'	1.873(9)
Si1'-C16'	1.869(8)	C16'-C17'	1.508(9)	C16'-C18'	1.518(9)
C16'-C19'	1.542(8)				

Table 18. Bond Angles in Compound 20, °

C6-C1-C2	118.3(3)	C6-C1-S1	118.6(2)	C2-C1-S1	123.0(2)
C3-C2-C1	121.8(3)	C3-C2-N1	116.7(3)	C1-C2-N1	121.5(3)
C4-C3-C2	118.8(3)	C3-C4-C5	120.8(3)	C6-C5-C4	120.1(3)
C5-C6-C1	120.2(3)	C9-C7-C8	119.7(3)	C9-C7-N2	111.1(2)
C8-C7-N2	59.1(2)	C9-C7-C11	113.8(3)	C8-C7-C11	120.5(3)
N2-C7-C11	121.6(2)	N2-C8-C7	61.5(2)	N2-C8-C12	116.1(3)
C7-C8-C12	125.4(3)	C10-C9-C7	178.4(4)	C8-C12-C13	110.8(3)
O5-C13-O5'	25.0(5)	O5-C13-C12	113.7(4)	O5'-C13-C12	100.8(4)
O2-N1-O1	125.6(3)	O2-N1-C2	116.7(3)	O1-N1-C2	117.6(3)
C8-N2-C7	59.41(18)	C8-N2-S1	121.61(19)	C7-N2-S1	121.03(18)
O3-S1-O4	119.33(13)	O3-S1-N2	113.58(14)	O4-S1-N2	106.27(13)
O3-S1-C1	107.59(13)	O4-S1-C1	107.88(15)	N2-S1-C1	100.44(12)
C13-O5-Si1	126.3(7)	O5-Si1-C15	104.9(7)	O5-Si1-C14	108.7(7)
C15-Si1-C14	112.5(7)	O5-Si1-C16	110.5(4)	C15-Si1-C16	112.6(6)
C14-Si1-C16	107.6(8)	C18-C16-C17	110.1(7)	C18-C16-C19	109.8(7)
C17-C16-C19	108.3(7)	C18-C16-Si1	111.3(8)	C17-C16-Si1	111.1(6)
C19-C16-Si1	106.1(8)	C13-O5'-Si1'	116.2(8)	O5'-Si1'-C15'	108.4(9)
O5'-Si1'-C14'	109.9(10)	C15'-Si1'-C14'	115.7(12)	O5'-Si1'-C16'	104.6(6)
C15'-Si1'-C16'	108.2(8)	C14'-Si1'-C16'	109.4(9)	C17'-C16'-C18'	111.9(8)
C17'-C16'-C19'	111.0(7)	C18'-C16'-C19'	110.4(7)	C17'-C16'-Si1'	108.3(8)
C18'-C16'-Si1'	108.5(8)	C19'-C16'-Si1'	106.6(8)		

ⁱBruker (2009) SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.

ⁱⁱBruker (2009) SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.

ⁱⁱⁱSheldrick, G.M. (2007) SADABS. University of Gottingen, Germany.

^{iv}Sheldrick, G.M. (2008) Acta Cryst. A64,112-122.

^vSheldrick, G.M. (2008) Acta Cryst. A64,112-122.

^{vi} $R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$

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

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

where n = the number of reflections and p = the number of parameters refined.

^{vii}“ORTEP-II: A Fortran Thermal Ellipsoid Plot Program for Crystal Structure Illustrations”.
C.K. Johnson (1976) ORNL-5138.