Inorganic Chemistry
including bioinorganic chemistry
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Table 1. Crystal data and structure refinement for SOL8NEU.

2a

Identification code	SOL8NEU
Empirical formula	$C_4H_{20}N_4Si_5$
Formula weight	264.69
Temperature	177(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 12.782(1) Å α = 90° b = 16.007(1) Å β = 109.04(1)° c = 15.631(1) Å γ = 90°
Volume	3023.2(4) $Å^3$
Z	8
Density (calculated)	1.163 Mg/m^3
Absorption coefficient	0.446 mm^{-1}
F(000)	1136
Crystal size	0.5 x 0.4 x 0.25 mm
θ range for data collection	3.01 to 25.96°
Index ranges	$0 \le h \le 15$, $0 \le k \le 19$, $-19 \le \ell \le 18$
Reflections collected	6215
Independent reflections	5916 (R_{int} = 0.0149)
Absorption correction	none
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5844 / 0 / 299
Goodness-of-fit on F^2	1.093
Final R indices [$I>2\sigma(I)$]	R1 = 0.0348, wR2 = 0.0924
R indices (all data)	R1 = 0.0485, wR2 = 0.1129
Largest diff. peak and hole	0.294 and -0.286 $eÅ^{-3}$

Table 2. Atomic coordinates und equivalent isotropic displacement parameters [Å^2] for SOL8NEU. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
Si(1)	0.24382(5)	0.64345(3)	0.13809(4)	0.03134(13)
Si(2)	0.19358(5)	0.81709(4)	0.18613(4)	0.0393(2)
Si(3)	0.33215(5)	0.75328(4)	0.30149(4)	0.0382(2)
Si(4)	0.28726(6)	0.52843(4)	0.00126(4)	0.0396(2)
Si(5)	0.17668(6)	0.46854(4)	0.07549(5)	0.0407(2)
N(1)	0.1667(2)	0.73362(11)	0.11298(12)	0.0396(4)
N(2)	0.3369(2)	0.66269(12)	0.24380(12)	0.0423(4)
N(3)	0.3071(2)	0.62169(12)	0.05914(13)	0.0427(5)
N(4)	0.1667(2)	0.55555(11)	0.13724(13)	0.0387(4)
C(1)	0.0801(3)	0.7398(2)	0.0240(2)	0.0652(8)
C(2)	0.4163(3)	0.5962(2)	0.2867(2)	0.0746(10)
C(3)	0.3812(3)	0.6857(2)	0.0419(2)	0.0760(10)
C(4)	0.1003(3)	0.5517(2)	0.1985(2)	0.0629(8)
Si(6)	0.25184(5)	1.12067(3)	-0.14291(4)	0.03146(13)
Si(7)	0.40046(6)	0.97926(4)	-0.15440(5)	0.0451(2)
Si(8)	0.27730(6)	0.94268(4)	-0.07989(5)	0.0481(2)
Si(9)	0.23537(6)	1.30590(4)	-0.12495(4)	0.0436(2)
Si(10)	0.11045(5)	1.25491(4)	-0.25749(4)	0.0379(2)
N(5)	0.3598(2)	1.08174(11)	-0.17336(14)	0.0399(4)
N(6)	0.2188(2)	1.04019(11)	-0.08368(13)	0.0399(4)
N(7)	0.2885(2)	1.21113(11)	-0.08067(12)	0.0377(4)
N(8)	0.1410(2)	1.15098(10)	-0.23460(12)	0.0351(4)
C(5)	0.4152(2)	1.1365(2)	-0.2207(2)	0.0545(7)
C(6)	0.1335(2)	1.0541(2)	-0.0409(2)	0.0563(7)
C(7)	0.3783(2)	1.2071(2)	0.0074(2)	0.0530(6)
C(8)	0.0797(2)	1.0868(2)	-0.2990(2)	0.0460(6)

Table 3. Bond lengths [Å] and angles [°] for SOL8NEU.

Si(1)-N(4)	1.716(2)	Si(1)-N(3)	1.717(2)
Si(1)-N(1)	1.720(2)	Si(1)-N(2)	1.720(2)
Si(2)-N(1)	1.719(2)	Si(2)-Si(3)	2.3126(9)
Si(2)-H(021)	1.44(3)	Si(2)-H(022)	1.43(3)
Si(3)-N(2)	1.719(2)	Si(3)-H(031)	1.38(2)
Si(3)-H(032)	1.33(3)	Si(4)-N(3)	1.721(2)
Si(4)-Si(5)	2.3094(9)	Si(4)-H(041)	1.40(3)
Si(4)-H(042)	1.43(3)	Si(5)-N(4)	1.723(2)
Si(5)-H(051)	1.41(3)	Si(5)-H(052)	1.37(3)
N(1)-C(1)	1.471(3)	N(2)-C(2)	1.472(3)
N(3)-C(3)	1.478(3)	N(4)-C(4)	1.473(3)
C(1)-H(11)	0.96	C(1)-H(12)	0.96
C(1)-H(13)	0.96	C(2)-H(21)	0.96
C(2)-H(22)	0.96	C(2)-H(23)	0.96
C(3)-H(31)	0.96	C(3)-H(32)	0.96
C(3)-H(33)	0.96	C(4)-H(41)	0.96
C(4)-H(42)	0.96	C(4)-H(43)	0.96
Si(6)-N(6)	1.718(2)	Si(6)-N(5)	1.717(2)
Si(6)-N(7)	1.722(2)	Si(6)-N(8)	1.724(2)
Si(7)-N(5)	1.717(2)	Si(7)-Si(8)	2.3182(10)
Si(7)-H(071)	1.39(3)	Si(7)-H(072)	1.36(3)
Si(8)-N(6)	1.723(2)	Si(8)-H(081)	1.40(3)
Si(8)-H(082)	1.41(3)	Si(9)-N(7)	1.713(2)
Si(9)-Si(10)	2.3129(9)	Si(9)-H(091)	1.32(3)
Si(9)-H(092)	1.46(3)	Si(10)-N(8)	1.720(2)
Si(10)-H(101)	1.40(2)	Si(10)-H(102)	1.37(3)
N(5)-C(5)	1.469(3)	N(6)-C(6)	1.470(3)
N(7)-C(7)	1.478(3)	N(8)-C(8)	1.472(3)
C(5)-H(51)	0.96	C(5)-H(52)	0.96
C(5)-H(53)	0.96	C(6)-H(61)	0.96
C(6)-H(62)	0.96	C(6)-H(63)	0.96
C(7)-H(71)	0.96	C(7)-H(72)	0.96
C(7)-H(73)	0.96	C(8)-H(81)	0.96
C(8)-H(82)	0.96	C(8)-H(83)	0.96

N(4)-Si(1)-N(3)	103.43(9)	N(4)-Si(1)-N(1)	113.67(10)
N(3)-Si(1)-N(1)	112.06(10)	N(4)-Si(1)-N(2)	111.72(10)
N(3)-Si(1)-N(2)	112.71(10)	N(1)-Si(1)-N(2)	103.56(9)
N(1)-Si(2)-Si(3)	96.40(7)	N(1)-Si(2)-H(021)	110.0(12)
Si(3)-Si(2)-H(021)	118.3(12)	N(1)-Si(2)-H(022)	113.9(12)
Si(3)-Si(2)-H(022)	110.3(12)	H(021)-Si(2)-H(022)	108(2)
N(2)-Si(3)-Si(2)	96.48(7)	N(2)-Si(3)-H(031)	111.5(10)
Si(2)-Si(3)-H(031)	115.6(10)	N(2)-Si(3)-H(032)	113.1(11)
Si(2)-Si(3)-H(032)	113.5(11)	H(031)-Si(3)-H(032)	107(2)
N(3)-Si(4)-Si(5)	96.04(7)	N(3)-Si(4)-H(041)	111.9(12)
Si(5)-Si(4)-H(041)	113.7(11)	N(3)-Si(4)-H(042)	113.1(11)
Si(5)-Si(4)-H(042)	114.4(11)	H(041)-Si(4)-H(042)	108(2)
N(4)-Si(5)-Si(4)	96.62(7)	N(4)-Si(5)-H(051)	109.0(12)
Si(4)-Si(5)-H(051)	111.0(12)	N(4)-Si(5)-H(052)	114.7(11)
Si(4)-Si(5)-H(052)	118.8(11)	H(051)-Si(5)-H(052)	106(2)
C(1)-N(1)-Si(1)	118.1(2)	C(1)-N(1)-Si(2)	120.1(2)
Si(1)-N(1)-Si(2)	121.69(11)	C(2)-N(2)-Si(3)	120.5(2)
C(2)-N(2)-Si(1)	117.8(2)	Si(3)-N(2)-Si(1)	121.54(11)
C(3)-N(3)-Si(1)	118.1(2)	C(3)-N(3)-Si(4)	119.9(2)
Si(1)-N(3)-Si(4)	122.04(11)	C(4)-N(4)-Si(1)	118.7(2)
C(4)-N(4)-Si(5)	119.6(2)	Si(1)-N(4)-Si(5)	121.33(11)
N(1)-C(1)-H(11)	109.87(13)	N(1)-C(1)-H(12)	109.2(2)
H(11)-C(1)-H(12)	109.5	N(1)-C(1)-H(13)	109.31(14)
H(11)-C(1)-H(13)	109.5	H(12)-C(1)-H(13)	109.5
N(2)-C(2)-H(21)	109.24(14)	N(2)-C(2)-H(22)	109.6(2)

H(21)-C(2)-H(22)	109.5	N(2)-C(2)-H(23)	109.5(2)
H(21)-C(2)-H(23)	109.5	H(22)-C(2)-H(23)	109.5
N(3)-C(3)-H(31)	109.56(14)	N(3)-C(3)-H(32)	109.8(2)
H(31)-C(3)-H(32)	109.5	N(3)-C(3)-H(33)	109.1(2)
H(31)-C(3)-H(33)	109.4	H(32)-C(3)-H(33)	109.5
N(4)-C(4)-H(41)	110.27(13)	N(4)-C(4)-H(42)	109.2(2)
H(41)-C(4)-H(42)	109.5	N(4)-C(4)-H(43)	108.9(2)
H(41)-C(4)-H(43)	109.5	H(42)-C(4)-H(43)	109.4
N(6)-Si(6)-N(5)	103.80(9)	N(6)-Si(6)-N(7)	113.30(10)
N(5)-Si(6)-N(7)	111.49(9)	N(6)-Si(6)-N(8)	112.29(9)
N(5)-Si(6)-N(8)	112.87(10)	N(7)-Si(6)-N(8)	103.39(8)
N(5)-Si(7)-Si(8)	96.40(7)	N(5)-Si(7)-H(071)	109.3(11)
Si(8)-Si(7)-H(071)	114.9(11)	N(5)-Si(7)-H(072)	110.9(13)
Si(8)-Si(7)-H(072)	116.9(13)	H(071)-Si(7)-H(072)	108(2)
N(6)-Si(8)-Si(7)	96.44(7)	N(6)-Si(8)-H(081)	112.3(13)
Si(7)-Si(8)-H(081)	115.8(13)	N(6)-Si(8)-H(082)	110.4(11)
Si(7)-Si(8)-H(082)	112.3(11)	H(081)-Si(8)-H(082)	109(2)
N(7)-Si(9)-Si(10)	96.68(7)	N(7)-Si(9)-H(091)	112.4(13)
Si(10)-Si(9)-H(091)	115.4(13)	N(7)-Si(9)-H(092)	111.9(11)
Si(10)-Si(9)-H(092)	114.2(11)	H(091)-Si(9)-H(092)	106(2)
N(8)-Si(10)-Si(9)	96.40(6)	N(8)-Si(10)-H(101)	112.1(10)
Si(9)-Si(10)-H(101)	113.9(10)	N(8)-Si(10)-H(102)	112.0(12)
Si(9)-Si(10)-H(102)	114.3(11)	H(101)-Si(10)-H(102)	108(2)
C(5)-N(5)-Si(7)	119.3(2)	C(5)-N(5)-Si(6)	119.1(2)
Si(7)-N(5)-Si(6)	121.61(11)	C(6)-N(6)-Si(6)	118.8(2)
C(6)-N(6)-Si(8)	120.0(2)	Si(6)-N(6)-Si(8)	121.16(11)
C(7)-N(7)-Si(9)	120.0(2)	C(7)-N(7)-Si(6)	118.4(2)
Si(9)-N(7)-Si(6)	121.14(10)	C(8)-N(8)-Si(10)	119.9(2)
C(8)-N(8)-Si(6)	118.8(2)	Si(10)-N(8)-Si(6)	120.97(10)
N(5)-C(5)-H(51)	110.29(13)	N(5)-C(5)-H(52)	109.1(2)
H(51)-C(5)-H(52)	109.5	N(5)-C(5)-H(53)	109.05(13)
H(51)-C(5)-H(53)	109.5	H(52)-C(5)-H(53)	109.4
N(6)-C(6)-H(61)	109.96(13)	N(6)-C(6)-H(62)	108.92(14)
H(61)-C(6)-H(62)	109.5	N(6)-C(6)-H(63)	109.54(14)
H(61)-C(6)-H(63)	109.5	H(62)-C(6)-H(63)	109.5
N(7)-C(7)-H(71)	109.62(12)	N(7)-C(7)-H(72)	109.38(13)
H(71)-C(7)-H(72)	109.5	N(7)-C(7)-H(73)	109.39(13)
H(71)-C(7)-H(73)	109.5	H(72)-C(7)-H(73)	109.5
N(8)-C(8)-H(81)	108.86(13)	N(8)-C(8)-H(82)	110.07(13)
H(81)-C(8)-H(82)	109.5	N(8)-C(8)-H(83)	109.47(12)
H(81)-C(8)-H(83)	109.4	H(82)-C(8)-H(83)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [Å^2] for SOL8NEU.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Si(1)	0.0385(3)	0.0266(3)	0.0276(3)	-0.0031(2)	0.0091(2)	-0.0005(2)
Si(2)	0.0473(4)	0.0252(3)	0.0429(3)	-0.0020(2)	0.0114(3)	0.0015(2)
Si(3)	0.0462(3)	0.0381(3)	0.0274(3)	-0.0066(2)	0.0082(2)	-0.0026(3)
Si(4)	0.0544(4)	0.0358(3)	0.0312(3)	-0.0056(2)	0.0174(3)	-0.0018(3)
Si(5)	0.0523(4)	0.0233(3)	0.0495(4)	-0.0013(2)	0.0206(3)	-0.0022(3)
N(1)	0.0436(10)	0.0298(9)	0.0352(10)	-0.0013(7)	-0.0013(8)	0.0019(8)
N(2)	0.0448(11)	0.0413(10)	0.0331(9)	-0.0058(8)	0.0022(8)	0.0137(8)
N(3)	0.0587(12)	0.0359(10)	0.0415(10)	-0.0102(8)	0.0271(9)	-0.0140(9)
N(4)	0.0509(11)	0.0296(9)	0.0433(10)	-0.0014(8)	0.0258(9)	-0.0027(8)
C(1)	0.071(2)	0.047(2)	0.049(2)	0.0024(12)	-0.0192(14)	0.0030(13)
C(2)	0.076(2)	0.071(2)	0.056(2)	-0.008(2)	-0.007(2)	0.038(2)
C(3)	0.105(3)	0.061(2)	0.086(2)	-0.023(2)	0.063(2)	-0.041(2)
C(4)	0.082(2)	0.048(2)	0.082(2)	-0.0040(14)	0.058(2)	-0.0047(14)
Si(6)	0.0384(3)	0.0213(3)	0.0357(3)	-0.0006(2)	0.0136(2)	0.0020(2)
Si(7)	0.0450(4)	0.0278(3)	0.0681(5)	-0.0015(3)	0.0259(3)	0.0056(3)
Si(8)	0.0525(4)	0.0275(3)	0.0690(5)	0.0122(3)	0.0265(4)	0.0050(3)
Si(9)	0.0561(4)	0.0239(3)	0.0427(3)	-0.0082(2)	0.0049(3)	0.0040(3)
Si(10)	0.0468(3)	0.0283(3)	0.0339(3)	0.0021(2)	0.0068(3)	0.0019(2)
N(5)	0.0450(10)	0.0254(9)	0.0565(12)	-0.0008(8)	0.0266(9)	-0.0012(8)
N(6)	0.0474(11)	0.0298(9)	0.0496(11)	0.0062(8)	0.0256(9)	0.0049(8)
N(7)	0.0458(10)	0.0281(9)	0.0328(9)	-0.0036(7)	0.0042(8)	0.0038(8)
N(8)	0.0429(10)	0.0251(8)	0.0350(9)	-0.0053(7)	0.0097(8)	-0.0020(7)
C(5)	0.066(2)	0.0376(13)	0.074(2)	-0.0014(12)	0.042(2)	-0.0091(12)
C(6)	0.067(2)	0.049(2)	0.068(2)	0.0055(13)	0.043(2)	0.0062(13)
C(7)	0.055(2)	0.0468(14)	0.0438(13)	-0.0018(11)	-0.0026(11)	0.0002(12)
C(8)	0.0561(14)	0.0379(12)	0.0417(12)	-0.0126(10)	0.0128(11)	-0.0107(11)

Table 5. Hydrogen coordinates and isotropic displacement parameters [$Å^2$] for SOL8NEU.

	x/a	y/b	z/c	U(eq)
H(021)	0.094(3)	0.842(2)	0.203(2)	0.075(9)
H(022)	0.236(3)	0.889(2)	0.154(2)	0.073(9)
H(031)	0.308(2)	0.738(2)	0.379(2)	0.047(7)
H(032)	0.427(2)	0.795(2)	0.326(2)	0.051(7)
H(041)	0.387(2)	0.486(2)	0.014(2)	0.062(8)
H(042)	0.235(2)	0.538(2)	-0.094(2)	0.060(8)
H(051)	0.234(2)	0.405(2)	0.135(2)	0.073(9)
H(052)	0.077(2)	0.435(2)	0.025(2)	0.052(7)
H(11)	0.0752(3)	0.6883(2)	-0.0084(2)	0.098
H(12)	0.0103(3)	0.7513(2)	0.0325(2)	0.098
H(13)	0.0980(3)	0.7844(2)	-0.0099(2)	0.098
H(21)	0.4070(3)	0.5504(2)	0.2453(2)	0.112
H(22)	0.4905(3)	0.6174(2)	0.3020(2)	0.112
H(23)	0.4031(3)	0.5774(2)	0.3406(2)	0.112
H(31)	0.3830(3)	0.7337(2)	0.0790(2)	0.114
H(32)	0.4546(3)	0.6633(2)	0.0557(2)	0.114
H(33)	0.3537(3)	0.7016(2)	-0.0207(2)	0.114
H(41)	0.1023(3)	0.6045(2)	0.2281(2)	0.094
H(42)	0.0252(3)	0.5381(2)	0.1641(2)	0.094
H(43)	0.1302(3)	0.5091(2)	0.2430(2)	0.094
H(071)	0.383(2)	0.939(2)	-0.237(2)	0.054(7)
H(072)	0.510(3)	0.974(2)	-0.106(2)	0.073(9)
H(081)	0.325(3)	0.913(2)	0.009(2)	0.078(10)
H(082)	0.197(2)	0.885(2)	-0.130(2)	0.062(8)
H(091)	0.192(2)	1.347(2)	-0.072(2)	0.071(9)
H(092)	0.320(2)	1.360(2)	-0.139(2)	0.069(9)
H(101)	0.131(2)	1.281(2)	-0.336(2)	0.050(7)
H(102)	0.002(2)	1.272(2)	-0.268(2)	0.059(8)
H(51)	0.4737(2)	1.1069(2)	-0.2336(2)	0.082
H(52)	0.3620(2)	1.1552(2)	-0.2763(2)	0.082
H(53)	0.4454(2)	1.1839(2)	-0.1831(2)	0.082
H(61)	0.1097(2)	1.1113(2)	-0.0484(2)	0.084
H(62)	0.0716(2)	1.0182(2)	-0.0690(2)	0.084
H(63)	0.1632(2)	1.0412(2)	0.0224(2)	0.084
H(71)	0.3901(2)	1.2615(2)	0.0346(2)	0.079
H(72)	0.3579(2)	1.1688(2)	0.0465(2)	0.079
H(73)	0.4451(2)	1.1882(2)	-0.0018(2)	0.079
H(81)	0.1069(2)	1.0327(2)	-0.2756(2)	0.069
H(82)	0.0021(2)	1.0904(2)	-0.3069(2)	0.069
H(83)	0.0909(2)	1.0951(2)	-0.3562(2)	0.069

Table 1. Crystal data and structure refinement for SOL6.

3

Identification code	SOL6
Empirical formula	$C_{13}H_{35}F_3N_4O_3SSi_3$
Formula weight	468.78
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 9.326(1) Å α = 90° b = 18.263(2) Å β = 105.37(1)° c = 15.089(1) Å γ = 90°
Volume	2478.0(4) $Å^3$
Z	4
Density (calculated)	1.257 Mg/m^3
Absorption coefficient	0.317 mm^{-1}
F(000)	1000
Crystal size	0.65 x 0.1 x 0.1 mm
θ range for data collection	3.01 to 24.98°
Index ranges	$-11 \le h \le 10$, $0 \le k \le 21$, $0 \le \ell \le 17$
Reflections collected	3496
Independent reflections	3377 (R_{int} = 0.0265)
Absorption correction	none
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3372 / 0 / 272
Goodness-of-fit on F^2	1.040
Final R indices [$I>2\sigma(I)$]	R1 = 0.0653, wR2 = 0.1435
R indices (all data)	R1 = 0.1221, wR2 = 0.1697
Largest diff. peak and hole	0.459 and -0.330 $eÅ^{-3}$

Table 2. Atomic coordinates und equivalent isotropic displacement parameters [$Å^2$] for SOL6. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
Si(1)	0.3172(2)	0.04785(8)	0.25637(10)	0.0332(4)
Si(2)	0.4074(2)	0.17249(14)	0.3847(2)	0.0730(7)
Si(3)	0.6073(2)	0.11247(13)	0.3536(2)	0.0687(7)
S	0.1418(2)	-0.09973(8)	-0.00136(11)	0.0435(4)
N(1)	0.2704(5)	0.1141(3)	0.3226(3)	0.0430(12)
N(2)	0.5068(5)	0.0429(3)	0.2864(3)	0.0392(11)
N(3)	0.2617(6)	0.0746(3)	0.1355(3)	0.0334(12)
N(4)	0.2243(6)	-0.0308(3)	0.2494(4)	0.0433(14)
C(1)	0.1112(6)	0.1220(4)	0.3269(4)	0.046(2)
C(11)	0.0975(7)	0.1028(4)	0.4217(5)	0.071(2)
C(12)	0.0503(7)	0.1969(4)	0.2970(5)	0.072(2)
C(2)	0.5815(6)	-0.0182(3)	0.2508(4)	0.047(2)
C(21)	0.6677(8)	-0.0662(5)	0.3300(6)	0.087(3)
C(22)	0.6849(8)	0.0097(4)	0.1966(5)	0.074(2)
C(3)	0.3432(7)	0.1363(3)	0.1019(4)	0.046(2)
C(31)	0.3382(8)	0.1238(4)	0.0026(4)	0.062(2)
C(32)	0.2793(9)	0.2092(3)	0.1155(6)	0.078(2)
C(4)	0.2265(7)	-0.0832(4)	0.3225(5)	0.060(2)
C(41)	0.0707(8)	-0.0949(5)	0.3325(6)	0.090(3)
C(42)	0.2920(9)	-0.1552(4)	0.3057(6)	0.094(3)
O(1)	0.2684(4)	-0.0521(2)	0.0233(3)	0.0537(11)
O(2)	0.0573(4)	-0.1041(3)	0.0641(3)	0.0618(13)
O(3)	0.0558(4)	-0.0948(3)	-0.0947(3)	0.0620(12)
C(01)	0.2273(10)	-0.1894(4)	0.0036(7)	0.081(2)
F(1)	0.1252(6)	-0.2411(2)	-0.0178(5)	0.126(2)
F(2)	0.3067(6)	-0.1929(3)	-0.0579(5)	0.121(2)
F(3)	0.3154(6)	-0.2024(3)	0.0846(5)	0.130(2)

Table 3. Bond lengths [Å] and angles [°] for SOL6.

Si(1)-N(4)	1.666(5)	Si(1)-N(1)	1.698(5)
Si(1)-N(2)	1.707(4)	Si(1)-N(3)	1.825(5)
Si(2)-N(1)	1.736(5)	Si(2)-Si(3)	2.315(3)
Si(2)-H(01)	1.57(6)	Si(2)-H(02)	1.29(6)
Si(3)-N(2)	1.737(5)	Si(3)-H(03)	1.57(7)
Si(3)-H(04)	1.39(8)	S-O(2)	1.419(4)
S-O(3)	1.427(4)	S-O(1)	1.434(4)
S-C(01)	1.815(8)	N(1)-C(1)	1.511(7)
N(2)-C(2)	1.489(7)	N(3)-C(3)	1.521(7)
N(3)-H(05)	0.95(5)	N(3)-H(06)	0.73(6)
N(4)-C(4)	1.457(8)	N(4)-H(07)	0.71(5)
C(1)-C(11)	1.511(9)	C(1)-C(12)	1.503(9)
C(1)-H(1)	0.96	C(11)-H(111)	0.96
C(11)-H(112)	0.96	C(11)-H(113)	0.95
C(12)-H(121)	0.96	C(12)-H(122)	0.95
C(12)-H(123)	0.96	C(2)-C(22)	1.508(9)
C(2)-C(21)	1.528(9)	C(2)-H(2A)	0.96
C(21)-H(211)	0.96	C(21)-H(212)	0.96
C(21)-H(213)	0.96	C(22)-H(221)	0.96
C(22)-H(222)	0.96	C(22)-H(223)	0.96
C(3)-C(32)	1.494(9)	C(3)-C(31)	1.503(8)
C(3)-H(3)	0.95	C(31)-H(311)	0.96
C(31)-H(312)	0.96	C(31)-H(313)	0.95
C(32)-H(321)	0.96	C(32)-H(322)	0.95
C(32)-H(323)	0.96	C(4)-C(42)	1.499(10)
C(4)-C(41)	1.515(9)	C(4)-H(4)	0.96
C(41)-H(411)	0.96	C(41)-H(412)	0.96
C(41)-H(413)	0.96	C(42)-H(421)	0.95
C(42)-H(422)	0.96	C(42)-H(423)	0.96
C(01)-F(3)	1.301(10)	C(01)-F(1)	1.318(9)
C(01)-F(2)	1.334(10)		

N(4)-Si(1)-N(1)	116.2(3)	N(4)-Si(1)-N(2)	117.1(3)
N(1)-Si(1)-N(2)	106.9(2)	N(4)-Si(1)-N(3)	99.3(3)
N(1)-Si(1)-N(3)	110.4(3)	N(2)-Si(1)-N(3)	106.2(2)
N(1)-Si(2)-Si(3)	96.7(2)	N(1)-Si(2)-H(01)	113(2)
Si(3)-Si(2)-H(01)	117(2)	N(1)-Si(2)-H(02)	116(3)
Si(3)-Si(2)-H(02)	117(3)	H(01)-Si(2)-H(02)	99(3)
N(2)-Si(3)-Si(2)	97.2(2)	N(2)-Si(3)-H(03)	113(2)
Si(2)-Si(3)-H(03)	110(2)	N(2)-Si(3)-H(04)	107(3)
Si(2)-Si(3)-H(04)	118(3)	H(03)-Si(3)-H(04)	111(4)
O(2)-S-O(3)	114.8(3)	O(2)-S-O(1)	115.1(3)
O(3)-S-O(1)	115.2(3)	O(2)-S-C(01)	103.9(4)
O(3)-S-C(01)	102.9(4)	O(1)-S-C(01)	102.3(3)
C(1)-N(1)-Si(1)	120.2(3)	C(1)-N(1)-Si(2)	120.6(4)
Si(1)-N(1)-Si(2)	119.2(3)	C(2)-N(2)-Si(1)	119.6(4)
C(2)-N(2)-Si(3)	121.8(4)	Si(1)-N(2)-Si(3)	118.5(3)
C(3)-N(3)-Si(1)	119.8(4)	C(3)-N(3)-H(05)	114(3)
Si(1)-N(3)-H(05)	101(3)	C(3)-N(3)-H(06)	106(5)
Si(1)-N(3)-H(06)	110(5)	H(05)-N(3)-H(06)	105(6)
C(4)-N(4)-Si(1)	128.0(5)	C(4)-N(4)-H(07)	115(5)
Si(1)-N(4)-H(07)	117(5)	C(11)-C(1)-C(12)	112.1(6)
C(11)-C(1)-N(1)	110.5(5)	C(12)-C(1)-N(1)	111.8(5)
C(11)-C(1)-H(1)	107.5(4)	C(12)-C(1)-H(1)	107.6(3)
N(1)-C(1)-H(1)	107.1(3)	C(1)-C(11)-H(111)	109.7(4)
C(1)-C(11)-H(112)	108.6(4)	H(111)-C(11)-H(112)	109.6
C(1)-C(11)-H(113)	110.3(3)	H(111)-C(11)-H(113)	109.3
H(112)-C(11)-H(113)	109.3	C(1)-C(12)-H(121)	110.3(4)
C(1)-C(12)-H(122)	109.6(3)	H(121)-C(12)-H(122)	109.4
C(1)-C(12)-H(123)	108.7(3)	H(121)-C(12)-H(123)	109.6

H(122)-C(12)-H(123)	109.3	N(2)-C(2)-C(22)	111.8(5)
N(2)-C(2)-C(21)	110.3(5)	C(22)-C(2)-C(21)	109.8(5)
N(2)-C(2)-H(2A)	108.9(3)	C(22)-C(2)-H(2A)	108.0(4)
C(21)-C(2)-H(2A)	108.1(4)	C(2)-C(21)-H(211)	110.0(4)
C(2)-C(21)-H(212)	110.0(4)	H(211)-C(21)-H(212)	109.2
C(2)-C(21)-H(213)	108.5(4)	H(211)-C(21)-H(213)	109.2
H(212)-C(21)-H(213)	109.9	C(2)-C(22)-H(221)	110.1(4)
C(2)-C(22)-H(222)	108.5(4)	H(221)-C(22)-H(222)	109.3
C(2)-C(22)-H(223)	109.7(4)	H(221)-C(22)-H(223)	109.4
H(222)-C(22)-H(223)	109.9	C(32)-C(3)-C(31)	111.4(6)
C(32)-C(3)-N(3)	111.2(5)	C(31)-C(3)-N(3)	109.5(5)
C(32)-C(3)-H(3)	108.3(4)	C(31)-C(3)-H(3)	109.0(4)
N(3)-C(3)-H(3)	107.4(3)	C(3)-C(31)-H(311)	110.2(3)
C(3)-C(31)-H(312)	109.1(4)	H(311)-C(31)-H(312)	109.8
C(3)-C(31)-H(313)	109.3(4)	H(311)-C(31)-H(313)	109.2
H(312)-C(31)-H(313)	109.2	C(3)-C(32)-H(321)	110.2(4)
C(3)-C(32)-H(322)	108.6(4)	H(321)-C(32)-H(322)	109.1
C(3)-C(32)-H(323)	109.7(4)	H(321)-C(32)-H(323)	109.4
H(322)-C(32)-H(323)	109.7	N(4)-C(4)-C(42)	111.9(6)
N(4)-C(4)-C(41)	110.3(6)	C(42)-C(4)-C(41)	109.8(6)
N(4)-C(4)-H(4)	107.8(3)	C(42)-C(4)-H(4)	109.0(4)
C(41)-C(4)-H(4)	108.0(4)	C(4)-C(41)-H(411)	109.7(4)
C(4)-C(41)-H(412)	107.7(4)	H(411)-C(41)-H(412)	109.7
C(4)-C(41)-H(413)	110.6(4)	H(411)-C(41)-H(413)	109.6
H(412)-C(41)-H(413)	109.5	C(4)-C(42)-H(421)	109.7(4)
C(4)-C(42)-H(422)	110.1(4)	H(421)-C(42)-H(422)	109.5
C(4)-C(42)-H(423)	108.7(4)	H(421)-C(42)-H(423)	109.3
H(422)-C(42)-H(423)	109.6	F(3)-C(01)-F(1)	109.6(8)
F(3)-C(01)-F(2)	108.4(7)	F(1)-C(01)-F(2)	107.1(8)
F(3)-C(01)-S	111.4(6)	F(1)-C(01)-S	110.8(6)
F(2)-C(01)-S	109.5(6)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$] for SOL6.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Si(1)	0.0306(8)	0.0382(9)	0.0285(8)	-0.0013(7)	0.0040(6)	-0.0049
Si(2)	0.0399(10)	0.097(2)	0.083(2)	-0.0553(14)	0.0164(10)	-0.0153
Si(3)	0.0327(9)	0.099(2)	0.0724(14)	-0.0409(13)	0.0106(9)	-0.0145
S	0.0353(8)	0.0420(9)	0.0472(9)	-0.0121(8)	0.0003(7)	0.0048
N(1)	0.031(2)	0.054(3)	0.044(3)	-0.020(2)	0.010(2)	-0.008(2
N(2)	0.030(2)	0.051(3)	0.034(2)	-0.004(2)	0.005(2)	0.000(2
N(3)	0.035(3)	0.028(3)	0.037(3)	0.003(2)	0.009(2)	-0.003(2
N(4)	0.045(3)	0.047(3)	0.035(3)	0.004(3)	0.005(3)	-0.008(2
C(1)	0.026(3)	0.063(4)	0.049(4)	-0.016(3)	0.008(3)	-0.002(3
C(11)	0.045(4)	0.109(6)	0.064(5)	-0.013(5)	0.026(4)	-0.001(4
C(12)	0.040(4)	0.083(5)	0.092(6)	-0.009(5)	0.018(4)	0.009(4
C(2)	0.043(3)	0.052(4)	0.048(4)	-0.004(3)	0.014(3)	0.007(3
C(21)	0.060(5)	0.093(6)	0.113(7)	0.052(5)	0.032(5)	0.028(4
C(22)	0.087(5)	0.078(5)	0.067(5)	0.007(4)	0.037(4)	0.035(5
C(3)	0.046(3)	0.039(4)	0.050(4)	0.017(3)	0.007(3)	-0.010(3
C(31)	0.077(5)	0.062(4)	0.054(4)	0.011(4)	0.031(4)	-0.016(4
C(32)	0.111(7)	0.033(4)	0.102(6)	0.007(4)	0.050(5)	-0.010(4
C(4)	0.056(4)	0.067(5)	0.056(4)	0.017(4)	0.013(3)	-0.009(4
C(41)	0.071(5)	0.095(6)	0.109(7)	0.041(6)	0.035(5)	-0.004(5
C(42)	0.079(6)	0.071(6)	0.130(8)	0.056(5)	0.026(5)	0.016(5
O(1)	0.048(2)	0.047(3)	0.061(3)	-0.014(2)	0.007(2)	-0.004(2
O(2)	0.043(2)	0.087(4)	0.055(3)	-0.015(3)	0.013(2)	-0.005(2
O(3)	0.050(3)	0.077(3)	0.051(3)	-0.006(3)	-0.001(2)	-0.003(2
C(01)	0.066(5)	0.052(5)	0.118(8)	-0.009(5)	0.016(6)	0.004(4
F(1)	0.106(4)	0.042(3)	0.231(7)	-0.018(3)	0.043(4)	-0.008(3
F(2)	0.085(3)	0.094(4)	0.192(6)	-0.064(4)	0.049(4)	0.014(3
F(3)	0.095(4)	0.095(4)	0.173(6)	0.042(4)	-0.012(4)	0.041(3

Table 5. Hydrogen coordinates and isotropic displacement parameters [$Å^2$] for SOL6.

	x/a	y/b	z/c	U(eq)
H(01)	0.382(6)	0.255(3)	0.353(4)	0.06(2)
H(02)	0.411(6)	0.181(3)	0.470(4)	0.06(2)
H(03)	0.687(7)	0.164(4)	0.299(4)	0.09(2)
H(04)	0.710(9)	0.079(4)	0.427(5)	0.11(3)
H(05)	0.267(5)	0.029(3)	0.107(3)	0.03(2)
H(06)	0.184(7)	0.084(4)	0.122(4)	0.05(2)
H(07)	0.185(6)	-0.043(3)	0.205(4)	0.03(2)
H(1)	0.0533(6)	0.0872(4)	0.2847(4)	0.070
H(111)	0.1361(7)	0.0545(4)	0.4381(5)	0.106
H(112)	0.1534(7)	0.1377(4)	0.4648(5)	0.106
H(113)	-0.0041(7)	0.1045(4)	0.4230(5)	0.106
H(121)	0.0586(7)	0.2072(4)	0.2361(5)	0.107
H(122)	-0.0516(7)	0.1992(4)	0.2974(5)	0.107
H(123)	0.1059(7)	0.2324(4)	0.3392(5)	0.107
H(2A)	0.5073(6)	-0.0479(3)	0.2108(4)	0.071
H(211)	0.6022(8)	-0.0845(5)	0.3640(6)	0.131
H(212)	0.7120(8)	-0.1067(5)	0.3066(6)	0.131
H(213)	0.7435(8)	-0.0371(5)	0.3697(6)	0.131
H(221)	0.6309(8)	0.0393(4)	0.1462(5)	0.111
H(222)	0.7607(8)	0.0387(4)	0.2365(5)	0.111
H(223)	0.7292(8)	-0.0309(4)	0.1734(5)	0.111
H(3)	0.4443(7)	0.1351(3)	0.1377(4)	0.069
H(311)	0.3908(8)	0.1619(4)	-0.0190(4)	0.093
H(312)	0.3827(8)	0.0773(4)	-0.0032(4)	0.093
H(313)	0.2371(8)	0.1235(4)	-0.0333(4)	0.093
H(321)	0.3335(9)	0.2475(3)	0.0955(6)	0.117
H(322)	0.1781(9)	0.2106(3)	0.0798(6)	0.117
H(323)	0.2841(9)	0.2159(3)	0.1793(6)	0.117
H(4)	0.2858(7)	-0.0628(4)	0.3789(5)	0.090
H(411)	0.0295(8)	-0.0489(5)	0.3442(6)	0.134
H(412)	0.0116(8)	-0.1151(5)	0.2759(6)	0.134
H(413)	0.0720(8)	-0.1282(5)	0.3820(6)	0.134
H(421)	0.3910(9)	-0.1479(4)	0.3011(6)	0.141
H(422)	0.2931(9)	-0.1884(4)	0.3552(6)	0.141
H(423)	0.2326(9)	-0.1753(4)	0.2491(6)	0.141