Table 1. Crystal data and structure refinement for **8a**.

Identification code	8a	
Empirical formula	C10 H21 F3 N4 O5 S Si	
Formula weight	394.46	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.900(5) Å	α= 81.211(13)°.
	b = 9.956(5) Å	β= 76.092(13)°.
	c = 11.399(7) Å	γ = 79.078(9)°.
Volume	849.1(9) Å^3	
Z	2	
Density (calculated)	1.543 Mg/m^3	
Absorption coefficient	0.322 mm^{-1}	
F(000)	412	
Crystal size	0.3 x 0.2 x 0.2 mm^3	
Theta range for data collection	1.85 to 28.56°.	
Index ranges	-10<=h<=10, -13<=k<=13, -15<=l<=15	
Reflections collected	8132	
Independent reflections	4255 [R(int) = 0.0616]	
Completeness to theta = 28.56°	98.2 %	
Absorption correction	Empirical	
Max. and min. transmission	1 and 0.46	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4255 / 0 / 217	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0828, wR2 = 0.2234	
R indices (all data)	R1 = 0.1121, wR2 = 0.2435	
Largest diff. peak and hole	1.487 and -0.665 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8a**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	U(eq)
Si(1)	2717(1)	7023(1)	7870(1)	19(1)
C(1)	3744(6)	5818(4)	8978(4)	32(1)
C(2)	7(5)	6570(5)	6702(3)	29(1)
C(3)	927(6)	4634(4)	8080(4)	32(1)
C(4)	-365(5)	7789(4)	9074(3)	21(1)
C(5)	-1537(5)	8614(4)	10002(3)	27(1)
C(6)	5046(5)	8678(5)	8406(4)	32(1)
C(7)	3374(6)	9787(4)	6905(4)	31(1)
C(8)	5170(5)	7064(4)	5969(3)	21(1)
C(9)	6266(5)	6422(4)	4903(4)	28(1)
N(1)	694(4)	6164(3)	7841(3)	21(1)
N(2)	-748(4)	6691(3)	8814(3)	23(1)
N(3)	5681(4)	7968(3)	6424(3)	25(1)
N(4)	4242(4)	8437(3)	7423(3)	22(1)
O(1)	1139(3)	8249(3)	8508(2)	20(1)
O(2)	3587(3)	6663(3)	6434(2)	20(1)
S(1)	2895(2)	7434(1)	2344(1)	31(1)
C(10)	1571(6)	8548(5)	3457(4)	32(1)
F(1)	1332(4)	9854(3)	2982(3)	47(1)
F(2)	2332(4)	8507(4)	4378(3)	54(1)
F(3)	-3(4)	8199(4)	3906(3)	58(1)
O(3)	2828(5)	6095(3)	2988(4)	52(1)
O(4)	1970(6)	7758(4)	1383(3)	53(1)
O(5)	4583(4)	7856(4)	2079(4)	52(1)

Table 3. Bond lengths [Å] and angles [°] for **8a**.

Si(1)-O(2)	1.680(3)	C(8)-N(3)	1.274(5)
Si(1)-O(1)	1.683(3)	C(8)-O(2)	1.346(4)
Si(1)-C(1)	1.831(4)	C(8)-C(9)	1.468(5)
Si(1)-N(4)	1.954(3)	N(1)-N(2)	1.466(4)
Si(1)-N(1)	1.959(3)	N(3)-N(4)	1.465(4)
C(2)-N(1)	1.496(5)	S(1)-O(4)	1.423(4)
C(3)-N(1)	1.490(5)	S(1)-O(5)	1.423(4)
C(4)-N(2)	1.282(5)	S(1)-O(3)	1.424(4)
C(4)-O(1)	1.336(4)	S(1)-C(10)	1.813(5)
C(4)-C(5)	1.468(5)	C(10)-F(3)	1.316(5)
C(6)-N(4)	1.483(5)	C(10)-F(2)	1.321(5)
C(7)-N(4)	1.493(5)	C(10)-F(1)	1.327(5)
O(2)-Si(1)-O(1)	134.33(13)	C(4)-N(2)-N(1)	107.3(3)
O(2)-Si(1)-C(1)	112.33(17)	C(8)-N(3)-N(4)	107.4(3)
O(1)-Si(1)-C(1)	113.34(17)	N(3)-N(4)-C(6)	107.7(3)
O(2)-Si(1)-N(4)	83.44(13)	N(3)-N(4)-C(7)	104.6(3)
O(1)-Si(1)-N(4)	86.23(14)	C(6)-N(4)-C(7)	108.7(3)
C(1)-Si(1)-N(4)	102.61(18)	N(3)-N(4)-Si(1)	106.5(2)
O(2)-Si(1)-N(1)	88.27(13)	C(6)-N(4)-Si(1)	115.0(3)
O(1)-Si(1)-N(1)	83.28(13)	C(7)-N(4)-Si(1)	113.7(2)
C(1)-Si(1)-N(1)	101.75(18)	C(4)-O(1)-Si(1)	113.4(2)
N(4)-Si(1)-N(1)	155.62(14)	C(8)-O(2)-Si(1)	113.5(2)
N(2)-C(4)-O(1)	121.4(3)	O(4)-S(1)-O(5)	115.4(3)
N(2)-C(4)-C(5)	122.5(3)	O(4)-S(1)-O(3)	115.4(2)
O(1)-C(4)-C(5)	116.1(3)	O(5)-S(1)-O(3)	114.6(2)
N(3)-C(8)-O(2)	121.5(3)	O(4)-S(1)-C(10)	102.5(2)
N(3)-C(8)-C(9)	121.8(3)	O(5)-S(1)-C(10)	103.5(2)
O(2)-C(8)-C(9)	116.7(3)	O(3)-S(1)-C(10)	102.8(2)
N(2)-N(1)-C(3)	106.5(3)	F(3)-C(10)-F(2)	107.5(4)
N(2)-N(1)-C(2)	105.2(3)	F(3)-C(10)-F(1)	107.3(4)
C(3)-N(1)-C(2)	107.6(3)	F(2)-C(10)-F(1)	106.6(4)
N(2)-N(1)-Si(1)	106.1(2)	F(3)-C(10)-S(1)	111.7(3)
C(3)-N(1)-Si(1)	116.4(2)	F(2)-C(10)-S(1)	111.6(3)
C(2)-N(1)-Si(1)	114.2(2)	F(1)-C(10)-S(1)	111.8(3)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si(1)	15(1)	20(1)	21(1)	-4(1)	-2(1)	-2(1)
C(1)	33(2)	31(2)	31(2)	1(2)	-14(2)	1(2)
C(2)	17(2)	43(2)	26(2)	-9(2)	-2(1)	-4(2)
C(3)	36(2)	22(2)	34(2)	-6(2)	3(2)	-10(2)
C(4)	18(2)	22(2)	20(2)	-6(1)	-1(1)	0(1)
C(5)	22(2)	28(2)	28(2)	-12(2)	5(1)	-2(2)
C(6)	22(2)	40(2)	38(2)	-14(2)	-4(2)	-11(2)
C(7)	30(2)	24(2)	38(2)	-5(2)	0(2)	-7(2)
C(8)	15(2)	24(2)	21(2)	-2(1)	2(1)	-2(1)
C(9)	21(2)	31(2)	31(2)	-11(2)	6(2)	-6(2)
N(1)	15(1)	23(2)	21(1)	-6(1)	3(1)	-5(1)
N(2)	17(1)	27(2)	22(1)	-9(1)	5(1)	-6(1)
N(3)	16(2)	28(2)	29(2)	-11(1)	5(1)	-7(1)
N(4)	13(1)	25(2)	29(2)	-10(1)	1(1)	-5(1)
O(1)	13(1)	20(1)	25(1)	-8(1)	3(1)	-2(1)
O(2)	16(1)	24(1)	20(1)	-7(1)	0(1)	-5(1)
S(1)	32(1)	26(1)	38(1)	-4(1)	-9(1)	-9(1)
C(10)	27(2)	35(2)	31(2)	1(2)	-4(2)	-4(2)
F(1)	51(2)	31(1)	50(2)	0(1)	-5(1)	3(1)
F(2)	60(2)	66(2)	37(2)	-10(1)	-18(1)	-1(2)
F(3)	27(1)	66(2)	68(2)	7(2)	9(1)	-10(1)
O(3)	56(2)	25(2)	74(3)	5(2)	-18(2)	-10(2)
O(4)	71(3)	53(2)	46(2)	-9(2)	-26(2)	-14(2)
O(5)	30(2)	53(2)	70(2)	-19(2)	8(2)	-15(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8a**.

	x	y	z	U(eq)
H(1A)	4794	6143	9073	48
H(1B)	4088	4906	8690	48
H(1C)	2900	5760	9763	48
H(2B)	-998	6102	6755	43
H(2C)	943	6306	6002	43
H(2D)	-375	7569	6605	43
H(3B)	-159	4317	8044	48
H(3C)	1181	4345	8890	48
H(3D)	1911	4233	7466	48
H(5A)	-2595	8189	10358	40
H(5B)	-1881	9548	9626	40
H(5C)	-916	8654	10641	40
H(6A)	5785	9398	8104	47
H(6B)	5775	7825	8666	47
H(6C)	4111	8969	9097	47
H(7A)	4207	10446	6701	47
H(7B)	2332	10137	7504	47
H(7C)	3014	9664	6168	47
H(9A)	7380	6790	4646	42
H(9B)	5636	6624	4238	42
H(9C)	6513	5424	5114	42

Table 1. Crystal data and structure refinement for **8c**.

Identification code	**8c**	
Empirical formula	C20 H25 F3 N4 O5 S Si	
Formula weight	518.59	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 28.606(4) Å	α= 90°.
	b = 12.2959(16) Å	β= 129.768(6)°.
	c = 18.410(3) Å	γ = 90°.
Volume	4977.3(12) $Å^3$	
Z	8	
Density (calculated)	1.384 Mg/m^3	
Absorption coefficient	0.238 mm^{-1}	
F(000)	2160	
Crystal size	0.3 x 0.3 x 0.1 mm^3	
Theta range for data collection	1.85 to 28.31°.	
Index ranges	-38<=h<=38, -14<=k<=16, -24<=l<=24	
Reflections collected	21494	
Independent reflections	6179 [R(int) = 0.0293]	
Completeness to theta = 28.31°	99.5 %	
Absorption correction	Empirical	
Max. and min. transmission	1 and 0.75	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6179 / 0 / 312	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.0573, wR2 = 0.1609	
R indices (all data)	R1 = 0.0706, wR2 = 0.1732	
Largest diff. peak and hole	0.997 and -0.818 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8c**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Si(1)	1699(1)	126(1)	851(1)	23(1)
C(1)	1524(1)	130(2)	1651(2)	36(1)
C(2)	2845(1)	-137(2)	1886(1)	27(1)
C(3)	3383(1)	-848(2)	2463(2)	34(1)
C(4)	3376(1)	-1858(2)	2122(2)	37(1)
C(5)	3883(1)	-2521(2)	2663(2)	49(1)
C(6)	4390(1)	-2188(3)	3550(3)	71(1)
C(7)	4390(1)	-1191(3)	3903(3)	87(1)
C(8)	3888(1)	-507(3)	3356(2)	62(1)
C(9)	2206(1)	2256(2)	1761(2)	34(1)
C(10)	2256(1)	1804(2)	525(2)	32(1)
C(11)	632(1)	392(2)	-709(1)	28(1)
C(12)	105(1)	1109(2)	-1349(1)	31(1)
C(13)	169(1)	2225(2)	-1224(2)	55(1)
C(14)	-335(1)	2893(3)	-1805(3)	72(1)
C(15)	-898(1)	2452(3)	-2504(2)	59(1)
C(16)	-963(1)	1341(2)	-2641(2)	46(1)
C(17)	-463(1)	669(2)	-2065(2)	37(1)
C(18)	1140(1)	-2039(2)	454(2)	45(1)
C(19)	1380(1)	-1489(2)	-542(2)	46(1)
C(20)	1444(1)	5037(2)	4623(2)	44(1)
F(1)	1423(1)	5573(3)	3991(2)	127(1)
F(2)	1248(1)	5753(3)	4885(2)	139(1)
F(3)	1045(1)	4263(2)	4180(2)	104(1)
N(1)	2881(1)	894(2)	1989(1)	30(1)
N(2)	2267(1)	1349(1)	1292(1)	25(1)
N(3)	579(1)	-637(2)	-686(1)	34(1)
N(4)	1193(1)	-1093(2)	10(1)	32(1)
O(1)	2308(1)	-638(1)	1240(1)	31(1)
O(2)	1180(1)	882(1)	-124(1)	28(1)
O(3)	2334(2)	3893(4)	5129(3)	148(2)

O(4)	2149(1)	4001(3)	6168(2)	118(1)
O(5)	2559(1)	5534(2)	5948(2)	76(1)
S(1)	2203(1)	4588(1)	5587(1)	36(1)

Table 3. Bond lengths [Å] and angles [°] for **8c**

Si(1)-O(1)	1.6844(15)	C(11)-C(12)	1.472(3)
Si(1)-O(2)	1.6964(14)	C(12)-C(13)	1.384(4)
Si(1)-C(1)	1.835(2)	C(12)-C(17)	1.390(3)
Si(1)-N(2)	1.9665(17)	C(13)-C(14)	1.387(4)
Si(1)-N(4)	1.9681(19)	C(14)-C(15)	1.375(4)
C(2)-N(1)	1.276(3)	C(15)-C(16)	1.380(4)
C(2)-O(1)	1.347(2)	C(16)-C(17)	1.382(3)
C(2)-C(3)	1.474(3)	C(18)-N(4)	1.485(3)
C(3)-C(4)	1.386(3)	C(19)-N(4)	1.500(3)
C(3)-C(8)	1.388(4)	C(20)-F(2)	1.291(4)
C(4)-C(5)	1.383(3)	C(20)-F(3)	1.297(3)
C(5)-C(6)	1.381(5)	C(20)-F(1)	1.305(4)
C(6)-C(7)	1.387(6)	C(20)-S(1)	1.800(3)
C(7)-C(8)	1.391(4)	N(1)-N(2)	1.470(2)
C(9)-N(2)	1.487(3)	N(3)-N(4)	1.469(2)
C(10)-N(2)	1.500(2)	O(3)-S(1)	1.408(3)
C(11)-N(3)	1.279(3)	O(4)-S(1)	1.378(2)
C(11)-O(2)	1.349(2)	O(5)-S(1)	1.403(2)
O(1)-Si(1)-O(2)	136.27(8)	N(1)-C(2)-C(3)	122.35(18)
O(1)-Si(1)-C(1)	113.54(10)	O(1)-C(2)-C(3)	116.09(18)
O(2)-Si(1)-C(1)	110.16(10)	C(4)-C(3)-C(8)	120.7(2)
O(1)-Si(1)-N(2)	83.94(7)	C(4)-C(3)-C(2)	119.9(2)
O(2)-Si(1)-N(2)	87.18(7)	C(8)-C(3)-C(2)	119.3(2)
C(1)-Si(1)-N(2)	104.14(9)	C(5)-C(4)-C(3)	119.7(2)
O(1)-Si(1)-N(4)	87.17(7)	C(6)-C(5)-C(4)	120.1(3)
O(2)-Si(1)-N(4)	83.04(7)	C(5)-C(6)-C(7)	120.0(3)
C(1)-Si(1)-N(4)	101.05(10)	C(6)-C(7)-C(8)	120.3(3)
N(2)-Si(1)-N(4)	154.78(8)	C(3)-C(8)-C(7)	119.0(3)
N(1)-C(2)-O(1)	121.56(17)	N(3)-C(11)-O(2)	121.12(17)

N(3)-C(11)-C(12)	122.46(18)	O(5)-S(1)-C(20)	105.36(13)
O(2)-C(11)-C(12)	116.41(18)	O(3)-S(1)-C(20)	102.16(17)
C(13)-C(12)-C(17)	119.6(2)		
C(13)-C(12)-C(11)	120.1(2)		
C(17)-C(12)-C(11)	120.3(2)		
C(12)-C(13)-C(14)	119.8(3)		
C(15)-C(14)-C(13)	120.3(3)		
C(14)-C(15)-C(16)	120.2(2)		
C(15)-C(16)-C(17)	119.9(2)		
C(16)-C(17)-C(12)	120.2(2)		
F(2)-C(20)-F(3)	108.6(3)		
F(2)-C(20)-F(1)	101.8(3)		
F(3)-C(20)-F(1)	106.8(3)		
F(2)-C(20)-S(1)	112.3(2)		
F(3)-C(20)-S(1)	114.55(18)		
F(1)-C(20)-S(1)	111.9(2)		
C(2)-N(1)-N(2)	108.09(16)		
N(1)-N(2)-C(9)	107.20(15)		
N(1)-N(2)-C(10)	104.90(14)		
C(9)-N(2)-C(10)	109.06(16)		
N(1)-N(2)-Si(1)	106.25(11)		
C(9)-N(2)-Si(1)	116.19(13)		
C(10)-N(2)-Si(1)	112.46(12)		
C(11)-N(3)-N(4)	107.78(16)		
N(3)-N(4)-C(18)	107.08(17)		
N(3)-N(4)-C(19)	106.19(17)		
C(18)-N(4)-C(19)	108.91(19)		
N(3)-N(4)-Si(1)	105.27(12)		
C(18)-N(4)-Si(1)	116.49(15)		
C(19)-N(4)-Si(1)	112.22(15)		
C(2)-O(1)-Si(1)	113.89(13)		
C(11)-O(2)-Si(1)	112.57(13)		
O(4)-S(1)-O(5)	118.35(19)		
O(4)-S(1)-O(3)	110.6(3)		
O(5)-S(1)-O(3)	113.3(3)		
O(4)-S(1)-C(20)	105.21(15)		

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for **8c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si(1)	18(1)	23(1)	24(1)	2(1)	12(1)	1(1)
C(1)	39(1)	41(1)	36(1)	-2(1)	27(1)	-7(1)
C(2)	20(1)	31(1)	27(1)	5(1)	14(1)	1(1)
C(3)	22(1)	36(1)	38(1)	12(1)	16(1)	4(1)
C(4)	34(1)	41(1)	41(1)	13(1)	26(1)	11(1)
C(5)	47(1)	47(2)	64(2)	24(1)	40(1)	20(1)
C(6)	32(1)	60(2)	87(2)	29(2)	22(2)	20(1)
C(7)	30(1)	70(2)	77(2)	14(2)	-5(1)	7(1)
C(8)	31(1)	46(2)	58(2)	3(1)	4(1)	3(1)
C(9)	35(1)	27(1)	37(1)	-4(1)	22(1)	-2(1)
C(10)	29(1)	34(1)	33(1)	9(1)	20(1)	1(1)
C(11)	20(1)	31(1)	27(1)	0(1)	11(1)	1(1)
C(12)	22(1)	36(1)	29(1)	7(1)	13(1)	5(1)
C(13)	30(1)	38(1)	61(2)	7(1)	13(1)	6(1)
C(14)	45(2)	40(2)	92(2)	19(2)	25(2)	17(1)
C(15)	31(1)	67(2)	62(2)	30(2)	23(1)	21(1)
C(16)	22(1)	69(2)	38(1)	19(1)	14(1)	5(1)
C(17)	23(1)	46(1)	34(1)	8(1)	14(1)	1(1)
C(18)	32(1)	25(1)	54(1)	5(1)	17(1)	-1(1)
C(19)	36(1)	46(1)	44(1)	-16(1)	20(1)	3(1)
C(20)	40(1)	35(1)	46(1)	6(1)	22(1)	4(1)
F(1)	83(2)	150(3)	74(1)	66(2)	16(1)	-16(2)
F(2)	75(2)	160(3)	125(2)	-35(2)	38(2)	56(2)
F(3)	46(1)	67(1)	96(2)	25(1)	-3(1)	-17(1)
N(1)	19(1)	32(1)	30(1)	5(1)	12(1)	0(1)
N(2)	20(1)	26(1)	25(1)	3(1)	12(1)	1(1)
N(3)	20(1)	31(1)	33(1)	0(1)	9(1)	2(1)
N(4)	21(1)	27(1)	35(1)	-1(1)	12(1)	4(1)
O(1)	20(1)	26(1)	35(1)	0(1)	12(1)	3(1)
O(2)	19(1)	27(1)	29(1)	3(1)	10(1)	1(1)

O(3)	73(2)	203(4)	110(2)	-70(3)	31(2)	48(2)
O(4)	58(1)	154(3)	70(2)	67(2)	7(1)	-37(2)
O(5)	53(1)	52(1)	67(1)	12(1)	13(1)	-21(1)
S(1)	32(1)	30(1)	40(1)	3(1)	19(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8c**.

	x	y	z	U(eq)
H(1A)	1686	-532	2036	55
H(1B)	1082	155	1280	55
H(1C)	1710	768	2064	55
H(4)	3023	-2095	1518	45
H(5)	3883	-3206	2424	59
H(6)	4739	-2643	3919	85
H(7)	4735	-975	4521	105
H(8)	3890	183	3591	75
H(9A)	2323	2001	2362	51
H(9B)	1784	2509	1350	51
H(9C)	2473	2856	1882	51
H(10A)	2606	2285	804	47
H(10B)	1879	2217	79	47
H(10C)	2274	1207	192	47
H(13)	557	2533	-742	66
H(14)	-291	3659	-1720	87
H(15)	-1242	2913	-2894	70
H(16)	-1351	1038	-3129	56
H(17)	-509	-96	-2159	44
H(18A)	964	-1802	742	67
H(18B)	1545	-2348	942	67
H(18C)	877	-2591	-28	67
H(19A)	1055	-1940	-1070	69
H(19B)	1753	-1921	-128	69
H(19C)	1454	-865	-786	69

Table 1. Crystal data and structure refinement for **8d**.

Identification code	**8d**	
Empirical formula	C15 H23 F3 N4 O5 S Si	
Formula weight	456.52	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.4678(15) Å	α= 89.784(5)°.
	b = 11.032(2) Å	β= 84.087(5)°.
	c = 11.517(2) Å	γ = 75.050(5)°.
Volume	1033.7(3) $Å^3$	
Z	2	
Density (calculated)	1.467 Mg/m^3	
Absorption coefficient	0.276 mm^{-1}	
F(000)	476	
Crystal size	0.3 x 0.3 x 0.1 mm^3	
Theta range for data collection	1.78 to 28.30°.	
Index ranges	-10<=h<=11, -14<=k<=14, -15<=l<=15	
Reflections collected	12650	
Independent reflections	5128 [R(int) = 0.0241]	
Completeness to theta = 28.30°	99.9 %	
Absorption correction	Empirical	
Max. and min. transmission	1 and 0.81	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5128 / 0 / 268	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0365, wR2 = 0.0941	
R indices (all data)	R1 = 0.0520, wR2 = 0.1016	
Largest diff. peak and hole	0.403 and -0.523 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8d**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Si(1)	2721(1)	7903(1)	8013(1)	17(1)
C(1)	-79(2)	8514(2)	7233(1)	22(1)
C(2)	-1365(2)	9460(2)	6701(2)	31(1)
C(3)	623(2)	6323(2)	8899(2)	31(1)
C(4)	2355(2)	5524(2)	7100(2)	31(1)
C(5)	4652(2)	7421(1)	9619(1)	21(1)
C(6)	5725(2)	6507(2)	10328(2)	30(1)
C(7)	2112(2)	9997(1)	9698(1)	24(1)
C(8)	4085(2)	10095(2)	8051(1)	26(1)
C(9)	4121(2)	7705(1)	6649(1)	20(1)
C(10)	5704(2)	6894(2)	6578(1)	27(1)
C(11)	6776(2)	6798(2)	5572(2)	34(1)
C(12)	6298(2)	7502(2)	4608(2)	33(1)
C(13)	4736(2)	8308(2)	4657(2)	34(1)
C(14)	3668(2)	8421(2)	5671(1)	27(1)
C(15)	1113(2)	6817(2)	3600(2)	35(1)
F(1)	2652(2)	6523(2)	3853(1)	70(1)
F(2)	418(1)	5960(1)	4082(1)	42(1)
F(3)	332(2)	7908(1)	4127(1)	65(1)
N(1)	95(2)	7335(1)	7114(1)	25(1)
N(2)	1444(2)	6685(1)	7780(1)	22(1)
N(3)	4731(2)	8559(1)	9512(1)	23(1)
N(4)	3413(2)	9224(1)	8823(1)	19(1)
O(1)	928(1)	8972(1)	7856(1)	22(1)
O(2)	3562(1)	6982(1)	9075(1)	21(1)
O(3)	-747(2)	7123(2)	1935(1)	55(1)
O(4)	1735(2)	7856(1)	1662(1)	58(1)
O(5)	1932(2)	5632(1)	1643(1)	40(1)
S(1)	993(1)	6867(1)	2026(1)	31(1)

Table 3. Bond lengths [Å] and angles [°] for **8d**.

Si(1)-O(2)	1.6833(11)	C(9)-C(10)	1.401(2)
Si(1)-O(1)	1.6911(11)	C(9)-C(14)	1.402(2)
Si(1)-C(9)	1.8453(15)	C(10)-C(11)	1.383(2)
Si(1)-N(2)	1.9645(13)	C(11)-C(12)	1.387(2)
Si(1)-N(4)	1.9747(13)	C(12)-C(13)	1.386(3)
C(1)-N(1)	1.276(2)	C(13)-C(14)	1.387(2)
C(1)-O(1)	1.3600(17)	C(15)-F(1)	1.322(2)
C(1)-C(2)	1.482(2)	C(15)-F(2)	1.329(2)
C(3)-N(2)	1.503(2)	C(15)-F(3)	1.330(2)
C(4)-N(2)	1.490(2)	C(15)-S(1)	1.8256(18)
C(5)-N(3)	1.279(2)	N(1)-N(2)	1.4699(17)
C(5)-O(2)	1.3532(17)	N(3)-N(4)	1.4729(16)
C(5)-C(6)	1.477(2)	O(3)-S(1)	1.4417(16)
C(7)-N(4)	1.5003(19)	O(4)-S(1)	1.4337(14)
C(8)-N(4)	1.4862(19)	O(5)-S(1)	1.4343(13)
O(2)-Si(1)-O(1)	137.05(6)	C(14)-C(9)-Si(1)	120.81(12)
O(2)-Si(1)-C(9)	112.09(6)	C(11)-C(10)-C(9)	120.90(15)
O(1)-Si(1)-C(9)	110.86(6)	C(10)-C(11)-C(12)	120.45(16)
O(2)-Si(1)-N(2)	87.54(5)	C(13)-C(12)-C(11)	119.62(16)
O(1)-Si(1)-N(2)	83.70(6)	C(12)-C(13)-C(14)	120.07(15)
C(9)-Si(1)-N(2)	102.21(6)	C(13)-C(14)-C(9)	121.11(15)
O(2)-Si(1)-N(4)	84.15(5)	F(1)-C(15)-F(2)	106.93(16)
O(1)-Si(1)-N(4)	88.03(5)	F(1)-C(15)-F(3)	108.33(16)
C(9)-Si(1)-N(4)	100.55(6)	F(2)-C(15)-F(3)	106.71(15)
N(2)-Si(1)-N(4)	157.24(6)	F(1)-C(15)-S(1)	111.80(13)
N(1)-C(1)-O(1)	121.32(13)	F(2)-C(15)-S(1)	111.05(12)
N(1)-C(1)-C(2)	122.63(14)	F(3)-C(15)-S(1)	111.76(13)
O(1)-C(1)-C(2)	116.05(13)	C(1)-N(1)-N(2)	107.92(12)
N(3)-C(5)-O(2)	121.09(13)	N(1)-N(2)-C(4)	107.17(11)
N(3)-C(5)-C(6)	123.06(13)	N(1)-N(2)-C(3)	105.31(12)
O(2)-C(5)-C(6)	115.85(13)	C(4)-N(2)-C(3)	109.02(12)
C(10)-C(9)-C(14)	117.83(14)	N(1)-N(2)-Si(1)	105.96(9)
C(10)-C(9)-Si(1)	121.26(11)	C(4)-N(2)-Si(1)	115.44(10)

C(3)-N(2)-Si(1)	113.22(10)	C(1)-O(1)-Si(1)	112.81(9)
C(5)-N(3)-N(4)	108.60(11)	C(5)-O(2)-Si(1)	114.42(9)
N(3)-N(4)-C(8)	107.46(11)	O(4)-S(1)-O(5)	114.80(9)
N(3)-N(4)-C(7)	105.11(11)	O(4)-S(1)-O(3)	115.37(10)
C(8)-N(4)-C(7)	108.04(12)	O(5)-S(1)-O(3)	115.03(10)
N(3)-N(4)-Si(1)	105.77(8)	O(4)-S(1)-C(15)	103.62(9)
C(8)-N(4)-Si(1)	115.45(9)	O(5)-S(1)-C(15)	102.28(8)
C(7)-N(4)-Si(1)	114.27(9)	O(3)-S(1)-C(15)	103.21(9)

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for **8d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si(1)	16(1)	16(1)	19(1)	0(1)	-3(1)	-4(1)
C(1)	17(1)	27(1)	24(1)	0(1)	-5(1)	-6(1)
C(2)	24(1)	28(1)	40(1)	1(1)	-14(1)	-3(1)
C(3)	32(1)	34(1)	32(1)	9(1)	-6(1)	-18(1)
C(4)	36(1)	19(1)	38(1)	-3(1)	-10(1)	-7(1)
C(5)	19(1)	22(1)	21(1)	-2(1)	-4(1)	-4(1)
C(6)	31(1)	25(1)	34(1)	0(1)	-15(1)	-1(1)
C(7)	21(1)	21(1)	26(1)	-5(1)	-2(1)	-2(1)
C(8)	31(1)	23(1)	28(1)	1(1)	-1(1)	-14(1)
C(9)	20(1)	19(1)	21(1)	-2(1)	-2(1)	-6(1)
C(10)	25(1)	25(1)	27(1)	3(1)	-1(1)	0(1)
C(11)	25(1)	32(1)	37(1)	2(1)	4(1)	2(1)
C(12)	31(1)	37(1)	27(1)	0(1)	6(1)	-8(1)
C(13)	33(1)	40(1)	26(1)	10(1)	-2(1)	-7(1)
C(14)	22(1)	30(1)	27(1)	5(1)	-3(1)	-3(1)
C(15)	43(1)	37(1)	28(1)	-3(1)	1(1)	-19(1)
F(1)	55(1)	115(1)	55(1)	-1(1)	-20(1)	-44(1)
F(2)	52(1)	41(1)	35(1)	12(1)	2(1)	-17(1)
F(3)	112(1)	43(1)	39(1)	-18(1)	22(1)	-29(1)
N(1)	25(1)	26(1)	29(1)	3(1)	-12(1)	-9(1)
N(2)	23(1)	20(1)	26(1)	2(1)	-8(1)	-8(1)
N(3)	18(1)	23(1)	28(1)	-1(1)	-9(1)	-3(1)
N(4)	17(1)	18(1)	21(1)	0(1)	-3(1)	-4(1)
O(1)	17(1)	20(1)	30(1)	-3(1)	-7(1)	-4(1)
O(2)	23(1)	19(1)	23(1)	2(1)	-7(1)	-7(1)
O(3)	44(1)	67(1)	47(1)	9(1)	-14(1)	2(1)
O(4)	95(1)	33(1)	45(1)	0(1)	27(1)	-26(1)
O(5)	53(1)	27(1)	36(1)	-7(1)	4(1)	-5(1)
S(1)	43(1)	23(1)	24(1)	1(1)	3(1)	-6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8d**.

	x	y	z	U(eq)
H(2A)	-2060	9036	6316	46
H(2B)	-844	9931	6125	46
H(2C)	-2040	10039	7311	46
H(3A)	41	7082	9358	46
H(3B)	1455	5799	9347	46
H(3C)	-162	5853	8721	46
H(4A)	1628	4969	7046	46
H(4B)	3309	5093	7493	46
H(4C)	2726	5748	6313	46
H(6A)	6462	6915	10685	45
H(6B)	6377	5801	9828	45
H(6C)	5047	6199	10943	45
H(7A)	1658	9441	10223	35
H(7B)	1232	10525	9290	35
H(7C)	2595	10532	10153	35
H(8A)	4461	10677	8528	40
H(8B)	3225	10570	7595	40
H(8C)	5011	9611	7520	40
H(10)	6046	6403	7231	33
H(11)	7846	6245	5540	40
H(12)	7037	7432	3917	39
H(13)	4397	8784	3995	40
H(14)	2611	8994	5704	32

Table 1. Crystal data and structure refinement for **12q**.

Identification code	**12q**	
Empirical formula	C15 H17 F9 N4 O5 S Si	
Formula weight	564.48	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 8.1265(6) Å	α= 90°.
	b = 17.6498(12) Å	β= 98.676(2)°.
	c = 16.1947(11) Å	γ = 90°.
Volume	2296.2(3) $Å^3$	
Z	4	
Density (calculated)	1.633 Mg/m^3	
Absorption coefficient	0.301 mm^{-1}	
F(000)	1144	
Crystal size	0.4 x 0.3 x 0.3 mm^3	
Theta range for data collection	13.81 to 26.39°.	
Index ranges	-9<=h<=9, 0<=k<=20, 0<=l<=20	
Reflections collected	12188	
Independent reflections	4598 [R(int) = 0.0975]	
Completeness to theta = 26.39°	60.7 %	
Absorption correction	Sadabs2	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2856 / 0 / 320	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0738, wR2 = 0.1723	
R indices (all data)	R1 = 0.1099, wR2 = 0.1970	
Largest diff. peak and hole	0.502 and -0.379 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **12q**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	2003(1)	2818(1)	9808(1)	13(1)
O(1)	972(4)	3613(2)	9285(2)	20(1)
C(1)	1279(6)	3690(3)	8523(3)	19(1)
C(2)	247(7)	4304(4)	8023(3)	23(1)
F(1)	324(6)	4256(3)	7214(2)	46(1)
F(2)	782(6)	4992(3)	8282(3)	49(1)
F(3)	-1335(5)	4254(3)	8120(3)	46(1)
N(1)	2336(5)	3324(3)	8178(2)	22(1)
N(2)	3260(5)	2822(3)	8811(2)	18(1)
O(2)	3512(4)	3457(2)	10319(2)	17(1)
C(3)	4987(6)	3150(3)	8945(3)	21(1)
C(4)	3355(6)	2069(3)	8400(3)	22(1)
C(5)	3119(6)	3750(3)	11015(3)	16(1)
C(6)	4356(7)	4323(4)	11427(3)	23(1)
F(4)	5911(4)	4085(3)	11460(2)	40(1)
F(5)	4195(6)	4970(3)	11000(3)	49(1)
F(6)	4117(5)	4484(3)	12203(2)	43(1)
N(3)	1841(5)	3593(3)	11344(2)	22(1)
N(4)	834(5)	3042(3)	10803(2)	18(1)
C(7)	-824(6)	3413(4)	10581(3)	24(1)
C(8)	625(7)	2374(4)	11342(3)	25(1)
C(9)	387(6)	2086(3)	9337(2)	16(1)
C(10)	503(6)	1303(3)	9533(3)	22(1)
C(11)	-590(8)	767(4)	9112(3)	32(1)
C(12)	-1853(7)	1006(4)	8493(3)	27(1)
C(13)	-2036(6)	1756(4)	8306(3)	25(1)
C(14)	-959(6)	2297(4)	8716(3)	22(1)
O(3)	3327(4)	2063(2)	10314(2)	18(1)
S(1)	4963(1)	1964(1)	10890(1)	19(1)
O(4)	4992(5)	2359(3)	11661(2)	26(1)

O(5)	6357(5)	2007(3)	10466(2)	31(1)
C(15)	4757(8)	959(4)	11153(4)	30(1)
F(7)	4571(6)	550(3)	10459(2)	45(1)
F(8)	6127(6)	742(3)	11635(3)	53(1)
F(9)	3454(5)	855(3)	11525(2)	39(1)

Table 3. Bond lengths [Å] and angles [°] for **12q**.

Si(1)-O(2)	1.775(4)	C(11)-C(12)	1.388(8)
Si(1)-O(1)	1.782(4)	C(12)-C(13)	1.363(9)
Si(1)-O(3)	1.828(4)	C(13)-C(14)	1.394(8)
Si(1)-C(9)	1.916(5)	O(3)-S(1)	1.515(3)
Si(1)-N(4)	2.029(4)	S(1)-O(5)	1.412(5)
Si(1)-N(2)	2.037(4)	S(1)-O(4)	1.426(4)
O(1)-C(1)	1.303(7)	S(1)-C(15)	1.838(8)
C(1)-N(1)	1.269(7)	C(15)-F(9)	1.308(9)
C(1)-C(2)	1.526(6)	C(15)-F(8)	1.316(7)
C(2)-F(3)	1.322(8)	C(15)-F(7)	1.325(9)
C(2)-F(1)	1.324(8)		
C(2)-F(2)	1.336(8)	O(2)-Si(1)-O(1)	87.92(18)
N(1)-N(2)	1.473(5)	O(2)-Si(1)-O(3)	86.32(17)
N(2)-C(4)	1.493(7)	O(1)-Si(1)-O(3)	172.09(18)
N(2)-C(3)	1.503(6)	O(2)-Si(1)-C(9)	175.52(18)
O(2)-C(5)	1.323(7)	O(1)-Si(1)-C(9)	95.56(19)
C(5)-N(3)	1.268(8)	O(3)-Si(1)-C(9)	90.5(2)
C(5)-C(6)	1.508(7)	O(2)-Si(1)-N(4)	83.07(16)
C(6)-F(4)	1.326(7)	O(1)-Si(1)-N(4)	88.93(18)
C(6)-F(6)	1.330(7)	O(3)-Si(1)-N(4)	95.74(17)
C(6)-F(5)	1.331(8)	C(9)-Si(1)-N(4)	94.16(18)
N(3)-N(4)	1.472(5)	O(2)-Si(1)-N(2)	88.49(17)
N(4)-C(8)	1.491(7)	O(1)-Si(1)-N(2)	82.93(17)
N(4)-C(7)	1.492(6)	O(3)-Si(1)-N(2)	91.50(16)
C(9)-C(14)	1.419(6)	C(9)-Si(1)-N(2)	94.72(18)
C(9)-C(10)	1.419(8)	N(4)-Si(1)-N(2)	168.5(2)
C(10)-C(11)	1.402(7)	C(1)-O(1)-Si(1)	112.8(4)

N(1)-C(1)-O(1)	127.1(4)
N(1)-C(1)-C(2)	118.8(5)
O(1)-C(1)-C(2)	114.1(5)
F(3)-C(2)-F(1)	107.7(4)
F(3)-C(2)-F(2)	107.4(6)
F(1)-C(2)-F(2)	107.9(6)
F(3)-C(2)-C(1)	110.9(5)
F(1)-C(2)-C(1)	112.0(5)
F(2)-C(2)-C(1)	110.7(4)
C(1)-N(1)-N(2)	107.9(4)
N(1)-N(2)-C(4)	106.3(3)
N(1)-N(2)-C(3)	103.7(4)
C(4)-N(2)-C(3)	107.3(4)
N(1)-N(2)-Si(1)	106.8(3)
C(4)-N(2)-Si(1)	114.6(3)
C(3)-N(2)-Si(1)	117.1(3)
C(5)-O(2)-Si(1)	114.0(3)
N(3)-C(5)-O(2)	126.2(4)
N(3)-C(5)-C(6)	119.6(4)
O(2)-C(5)-C(6)	114.1(4)
F(4)-C(6)-F(6)	107.7(4)
F(4)-C(6)-F(5)	108.1(5)
F(6)-C(6)-F(5)	106.8(5)
F(4)-C(6)-C(5)	111.9(5)
F(6)-C(6)-C(5)	112.2(5)
F(5)-C(6)-C(5)	109.8(4)
C(5)-N(3)-N(4)	108.2(4)
N(3)-N(4)-C(8)	106.0(3)
N(3)-N(4)-C(7)	104.7(4)
C(8)-N(4)-C(7)	108.0(4)
N(3)-N(4)-Si(1)	108.5(3)
C(8)-N(4)-Si(1)	114.8(4)
C(7)-N(4)-Si(1)	114.1(3)
C(14)-C(9)-C(10)	115.6(5)
C(14)-C(9)-Si(1)	120.9(4)
C(10)-C(9)-Si(1)	123.3(3)
C(11)-C(10)-C(9)	122.2(4)
C(12)-C(11)-C(10)	119.5(6)
C(13)-C(12)-C(11)	120.0(5)
C(12)-C(13)-C(14)	121.3(4)
C(13)-C(14)-C(9)	121.3(5)
S(1)-O(3)-Si(1)	139.7(3)
O(5)-S(1)-O(4)	119.4(3)
O(5)-S(1)-O(3)	112.9(2)
O(4)-S(1)-O(3)	112.4(2)
O(5)-S(1)-C(15)	105.7(3)
O(4)-S(1)-C(15)	105.0(3)
O(3)-S(1)-C(15)	98.7(3)
F(9)-C(15)-F(8)	110.9(5)
F(9)-C(15)-F(7)	108.5(6)
F(8)-C(15)-F(7)	108.8(6)
F(9)-C(15)-S(1)	110.6(5)
F(8)-C(15)-S(1)	108.7(5)
F(7)-C(15)-S(1)	109.4(4)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	10(1)	16(1)	17(1)	0(1)	7(1)	-2(1)
O(1)	18(2)	20(3)	22(2)	5(1)	8(1)	0(1)
C(1)	20(2)	12(3)	25(2)	0(2)	5(2)	2(2)
C(2)	25(3)	21(4)	24(2)	4(2)	8(2)	5(2)
F(1)	58(2)	53(4)	29(2)	11(2)	11(1)	27(2)
F(2)	65(3)	14(3)	62(2)	3(2)	-9(2)	4(2)
F(3)	32(2)	51(4)	55(2)	21(2)	6(2)	15(2)
N(1)	21(2)	24(3)	21(2)	2(1)	4(2)	3(2)
N(2)	16(2)	15(3)	25(2)	3(1)	6(1)	1(2)
O(2)	16(2)	17(2)	21(1)	-1(1)	11(1)	-1(1)
C(3)	15(2)	25(4)	25(2)	3(2)	10(2)	-3(2)
C(4)	18(2)	25(4)	24(2)	-2(2)	13(2)	5(2)
C(5)	15(2)	15(3)	19(2)	-3(2)	9(2)	4(2)
C(6)	22(3)	18(4)	31(2)	-9(2)	7(2)	2(2)
F(4)	16(2)	49(3)	57(2)	-25(2)	7(1)	-3(1)
F(5)	57(2)	26(3)	61(2)	6(2)	-5(2)	-15(2)
F(6)	37(2)	59(4)	35(2)	-25(2)	12(1)	-15(2)
N(3)	16(2)	27(3)	22(2)	-6(2)	6(2)	-1(2)
N(4)	13(2)	21(3)	21(2)	0(1)	7(1)	-5(2)
C(7)	12(2)	33(4)	30(2)	-3(2)	9(2)	0(2)
C(8)	26(3)	34(4)	18(2)	2(2)	16(2)	-7(2)
C(9)	11(2)	22(3)	18(2)	-2(2)	11(2)	2(2)
C(10)	22(2)	18(4)	24(2)	1(2)	3(2)	-4(2)
C(11)	35(3)	23(4)	34(3)	4(2)	-2(2)	-7(2)
C(12)	27(3)	18(4)	35(2)	-5(2)	2(2)	-9(2)
C(13)	16(2)	32(4)	27(2)	-1(2)	2(2)	-2(2)
C(14)	10(2)	31(4)	27(2)	-2(2)	9(2)	2(2)
O(3)	14(2)	17(2)	23(1)	1(1)	7(1)	2(1)
S(1)	16(1)	20(1)	22(1)	2(1)	6(1)	0(1)
O(4)	29(2)	25(3)	23(2)	1(1)	5(1)	-2(1)

O(5)	14(2)	39(3)	41(2)	6(2)	11(1)	0(2)
C(15)	30(3)	27(5)	34(3)	2(2)	5(2)	3(2)
F(7)	67(3)	19(3)	51(2)	-4(2)	13(2)	9(2)
F(8)	40(2)	45(4)	69(2)	25(2)	-12(2)	8(2)
F(9)	43(2)	28(3)	51(2)	10(1)	23(2)	-5(2)

Table 1. Crystal data and structure refinement for **13n**.

Identification code	**13n**	
Empirical formula	C20 H22 F6 N4 O8 S2 Si	
Formula weight	652.63	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 16.466(5) Å	α= 90°.
	b = 8.193(3) Å	β= 102.427(7)°.
	c = 20.861(7) Å	γ = 90°.
Volume	2748.3(15) $Å^3$	
Z	4	
Density (calculated)	1.577 Mg/m^3	
Absorption coefficient	0.330 mm^{-1}	
F(000)	1336	
Crystal size	0.1 x 0.2 x 0.2 mm^3	
Theta range for data collection	2.53 to 23.26°.	
Index ranges	-18<=h<=18, -9<=k<=9, -23<=l<=23	
Reflections collected	26602	
Independent reflections	3920 [R(int) = 0.0500]	
Completeness to theta = 23.26°	99.3 %	
Absorption correction	Empirical	
Max. and min. transmission	1 and 0.66	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3920 / 0 / 374	
Goodness-of-fit on F^2	1.086	
Final R indices [I>2sigma(I)]	R1 = 0.0506, wR2 = 0.1202	
R indices (all data)	R1 = 0.0642, wR2 = 0.1258	
Largest diff. peak and hole	0.372 and -0.424 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **13n**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Si(1)	7801(1)	580(1)	305(1)	23(1)
S(1)	7850(1)	3729(1)	1179(1)	36(1)
S(2)	6243(1)	1620(1)	-690(1)	32(1)
C(1)	6784(3)	-2244(5)	459(2)	33(1)
C(2)	6406(2)	156(5)	998(2)	32(1)
C(3)	8427(2)	-1125(5)	1322(2)	27(1)
C(4)	9133(2)	-1620(5)	1843(2)	31(1)
C(5)	9045(3)	-1734(6)	2492(2)	44(1)
C(6)	9696(3)	-2249(7)	2979(2)	52(1)
C(7)	10444(3)	-2681(7)	2818(3)	55(1)
C(8)	10545(3)	-2501(7)	2186(3)	52(1)
C(9)	9894(3)	-1982(6)	1700(2)	39(1)
C(10)	8402(4)	3470(7)	2030(2)	54(1)
C(11)	8348(3)	3187(5)	-505(2)	33(1)
C(12)	9453(2)	1966(5)	296(2)	30(1)
C(13)	8203(2)	-626(5)	-726(2)	25(1)
C(14)	8161(2)	-1878(5)	-1240(2)	28(1)
C(15)	8700(3)	-1811(6)	-1674(2)	36(1)
C(16)	8625(3)	-2941(6)	-2172(2)	44(1)
C(17)	8011(3)	-4114(6)	-2248(2)	46(1)
C(18)	7479(3)	-4199(6)	-1819(2)	42(1)
C(19)	7560(3)	-3081(5)	-1315(2)	36(1)
C(20)	5655(3)	3459(6)	-578(3)	49(1)
F(1)	9191(2)	3179(5)	2057(2)	90(1)
F(2)	8323(3)	4803(4)	2359(2)	94(1)
F(3)	8096(2)	2248(4)	2310(1)	68(1)
F(4)	6119(2)	4766(4)	-558(2)	73(1)
F(5)	5373(2)	3358(4)	-35(2)	66(1)
F(6)	5013(2)	3572(4)	-1081(2)	74(1)
N(1)	7110(2)	-677(4)	789(2)	27(1)
N(2)	7677(2)	-1197(4)	1403(2)	30(1)

N(3)	8621(2)	1641(4)	-136(1)	25(1)
N(4)	8767(2)	491(4)	-637(2)	28(1)
O(1)	8597(2)	-593(3)	756(1)	26(1)
O(2)	7996(2)	2087(3)	945(1)	30(1)
O(3)	8293(2)	4938(4)	905(2)	49(1)
O(4)	7003(2)	4003(4)	1200(2)	53(1)
O(5)	6935(2)	1819(3)	-79(1)	26(1)
O(6)	6528(2)	1855(5)	-1278(1)	52(1)
O(7)	5714(2)	282(4)	-644(1)	40(1)
O(8)	7623(2)	-694(3)	-369(1)	27(1)

Table 3. Bond lengths [Å] and angles [°] for **13n**.

Si(1)-O(8)	1.724(3)	C(6)-C(7)	1.392(7)
Si(1)-O(1)	1.731(3)	C(7)-C(8)	1.372(7)
Si(1)-O(5)	1.793(3)	C(8)-C(9)	1.374(6)
Si(1)-O(2)	1.796(3)	C(10)-F(1)	1.310(6)
Si(1)-N(1)	1.967(3)	C(10)-F(2)	1.312(6)
Si(1)-N(3)	1.989(3)	C(10)-F(3)	1.313(6)
S(1)-O(3)	1.421(3)	C(11)-N(3)	1.500(5)
S(1)-O(4)	1.422(3)	C(12)-N(3)	1.493(5)
S(1)-O(2)	1.469(3)	C(13)-N(4)	1.289(5)
S(1)-C(10)	1.823(5)	C(13)-O(8)	1.332(4)
S(2)-O(7)	1.416(3)	C(13)-C(14)	1.473(6)
S(2)-O(6)	1.418(3)	C(14)-C(19)	1.381(6)
S(2)-O(5)	1.524(3)	C(14)-C(15)	1.399(6)
S(2)-C(20)	1.833(5)	C(15)-C(16)	1.378(6)
C(1)-N(1)	1.501(5)	C(16)-C(17)	1.380(7)
C(2)-N(1)	1.488(5)	C(17)-C(18)	1.382(7)
C(3)-N(2)	1.284(5)	C(18)-C(19)	1.379(6)
C(3)-O(1)	1.343(5)	C(20)-F(4)	1.311(6)
C(3)-C(4)	1.467(6)	C(20)-F(5)	1.316(6)
C(4)-C(9)	1.383(6)	C(20)-F(6)	1.322(6)
C(4)-C(5)	1.395(6)	N(1)-N(2)	1.477(4)
C(5)-C(6)	1.375(7)	N(3)-N(4)	1.467(4)

O(8)-Si(1)-O(1)	94.76(14)	C(7)-C(8)-C(9)	120.4(5)
O(8)-Si(1)-O(5)	89.95(13)	C(8)-C(9)-C(4)	120.4(4)
O(1)-Si(1)-O(5)	173.60(13)	F(1)-C(10)-F(2)	109.8(5)
O(8)-Si(1)-O(2)	173.62(14)	F(1)-C(10)-F(3)	108.3(5)
O(1)-Si(1)-O(2)	89.09(13)	F(2)-C(10)-F(3)	108.1(4)
O(5)-Si(1)-O(2)	86.62(13)	F(1)-C(10)-S(1)	110.2(3)
O(8)-Si(1)-N(1)	94.98(14)	F(2)-C(10)-S(1)	109.1(4)
O(1)-Si(1)-N(1)	83.37(13)	F(3)-C(10)-S(1)	111.3(4)
O(5)-Si(1)-N(1)	91.91(13)	N(4)-C(13)-O(8)	122.0(4)
O(2)-Si(1)-N(1)	90.51(14)	N(4)-C(13)-C(14)	121.2(3)
O(8)-Si(1)-N(3)	84.29(13)	O(8)-C(13)-C(14)	116.8(3)
O(1)-Si(1)-N(3)	89.08(13)	C(19)-C(14)-C(15)	119.5(4)
O(5)-Si(1)-N(3)	95.71(13)	C(19)-C(14)-C(13)	120.0(4)
O(2)-Si(1)-N(3)	90.70(13)	C(15)-C(14)-C(13)	120.4(4)
N(1)-Si(1)-N(3)	172.34(14)	C(16)-C(15)-C(14)	119.8(4)
O(3)-S(1)-O(4)	119.5(2)	C(15)-C(16)-C(17)	119.9(4)
O(3)-S(1)-O(2)	111.71(18)	C(16)-C(17)-C(18)	120.8(4)
O(4)-S(1)-O(2)	112.78(19)	C(19)-C(18)-C(17)	119.3(5)
O(3)-S(1)-C(10)	106.3(2)	C(18)-C(19)-C(14)	120.7(4)
O(4)-S(1)-C(10)	106.0(2)	F(4)-C(20)-F(5)	109.6(5)
O(2)-S(1)-C(10)	97.7(2)	F(4)-C(20)-F(6)	109.2(4)
O(7)-S(2)-O(6)	119.2(2)	F(5)-C(20)-F(6)	108.6(4)
O(7)-S(2)-O(5)	112.70(17)	F(4)-C(20)-S(2)	110.8(3)
O(6)-S(2)-O(5)	112.38(17)	F(5)-C(20)-S(2)	110.6(3)
O(7)-S(2)-C(20)	106.2(2)	F(6)-C(20)-S(2)	108.1(4)
O(6)-S(2)-C(20)	106.3(2)	N(2)-N(1)-C(2)	105.4(3)
O(5)-S(2)-C(20)	97.25(19)	N(2)-N(1)-C(1)	104.3(3)
N(2)-C(3)-O(1)	121.4(3)	C(2)-N(1)-C(1)	107.6(3)
N(2)-C(3)-C(4)	121.3(3)	N(2)-N(1)-Si(1)	105.6(2)
O(1)-C(3)-C(4)	117.3(3)	C(2)-N(1)-Si(1)	118.9(3)
C(9)-C(4)-C(5)	118.9(4)	C(1)-N(1)-Si(1)	113.7(2)
C(9)-C(4)-C(3)	120.6(4)	C(3)-N(2)-N(1)	108.5(3)
C(5)-C(4)-C(3)	120.5(4)	N(4)-N(3)-C(12)	105.9(3)
C(6)-C(5)-C(4)	120.8(5)	N(4)-N(3)-C(11)	104.6(3)
C(5)-C(6)-C(7)	119.2(4)	C(12)-N(3)-C(11)	107.0(3)
C(8)-C(7)-C(6)	120.1(4)	N(4)-N(3)-Si(1)	106.4(2)

C(12)-N(3)-Si(1)	115.2(2)	S(1)-O(2)-Si(1)	149.43(19)
C(11)-N(3)-Si(1)	116.7(2)	S(2)-O(5)-Si(1)	133.85(17)
C(13)-N(4)-N(3)	109.5(3)	C(13)-O(8)-Si(1)	114.5(2)
C(3)-O(1)-Si(1)	112.4(2)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **13n**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si(1)	20(1)	28(1)	20(1)	1(1)	5(1)	2(1)
S(1)	40(1)	35(1)	35(1)	-2(1)	12(1)	0(1)
S(2)	26(1)	42(1)	27(1)	4(1)	1(1)	3(1)
C(1)	29(2)	31(2)	37(2)	4(2)	7(2)	-5(2)
C(2)	22(2)	42(3)	33(2)	3(2)	10(2)	1(2)
C(3)	26(2)	30(2)	26(2)	5(2)	8(2)	0(2)
C(4)	28(2)	31(2)	30(2)	8(2)	1(2)	-7(2)
C(5)	36(3)	61(3)	36(3)	10(2)	9(2)	-11(2)
C(6)	49(3)	72(4)	31(3)	14(2)	0(2)	-21(3)
C(7)	41(3)	65(4)	51(3)	26(3)	-9(2)	-8(3)
C(8)	32(3)	63(3)	58(3)	14(3)	3(2)	10(3)
C(9)	32(3)	45(3)	39(3)	6(2)	4(2)	6(2)
C(10)	73(4)	54(3)	38(3)	-7(3)	20(3)	-13(3)
C(11)	36(2)	30(2)	34(2)	12(2)	11(2)	2(2)
C(12)	24(2)	37(2)	29(2)	-2(2)	6(2)	-5(2)
C(13)	26(2)	31(2)	19(2)	6(2)	4(2)	7(2)
C(14)	28(2)	35(2)	19(2)	2(2)	1(2)	8(2)
C(15)	33(2)	52(3)	24(2)	-7(2)	5(2)	3(2)
C(16)	44(3)	62(3)	27(2)	-6(2)	10(2)	13(3)
C(17)	53(3)	49(3)	30(2)	-12(2)	-1(2)	14(3)
C(18)	49(3)	33(3)	41(3)	-7(2)	0(2)	5(2)
C(19)	38(3)	38(3)	30(2)	2(2)	4(2)	4(2)
C(20)	30(3)	46(3)	65(3)	16(3)	-2(2)	1(2)
F(1)	58(2)	142(4)	59(2)	-5(2)	-13(2)	-11(2)
F(2)	174(4)	62(2)	48(2)	-30(2)	28(2)	-29(2)

F(3)	106(3)	61(2)	39(2)	1(2)	20(2)	-7(2)
F(4)	51(2)	39(2)	123(3)	18(2)	8(2)	4(2)
F(5)	55(2)	62(2)	90(2)	1(2)	32(2)	22(2)
F(6)	38(2)	72(2)	98(2)	31(2)	-15(2)	13(2)
N(1)	20(2)	35(2)	27(2)	6(2)	5(1)	2(2)
N(2)	30(2)	36(2)	25(2)	4(2)	5(2)	-1(2)
N(3)	26(2)	28(2)	21(2)	0(1)	6(1)	2(2)
N(4)	28(2)	34(2)	22(2)	-1(2)	7(1)	1(2)
O(1)	22(1)	32(2)	27(1)	6(1)	8(1)	4(1)
O(2)	24(2)	43(2)	22(1)	0(1)	3(1)	-3(1)
O(3)	63(2)	36(2)	55(2)	-1(2)	27(2)	-4(2)
O(4)	44(2)	48(2)	70(2)	-3(2)	22(2)	9(2)
O(5)	24(1)	32(2)	21(1)	-1(1)	2(1)	5(1)
O(6)	44(2)	86(3)	24(2)	4(2)	2(1)	-6(2)
O(7)	31(2)	43(2)	42(2)	3(1)	-3(1)	0(1)
O(8)	25(1)	30(2)	26(1)	-3(1)	8(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **13n**.

	x	y	z	U(eq)
H(1A)	7248	-2891	370	49
H(1B)	6393	-2002	45	49
H(1C)	6497	-2863	747	49
H(2A)	6183	-557	1296	48
H(2B)	5968	399	611	48
H(2C)	6603	1176	1224	48
H(5)	8530	-1453	2598	53
H(6)	9635	-2309	3421	62
H(7)	10887	-3100	3146	66
H(8)	11067	-2738	2083	63
H(9)	9969	-1871	1263	47
H(11A)	8794	3581	-710	49
H(11B)	8225	4016	-201	49
H(11C)	7849	2974	-845	49

H(12A)	9678	951	512	45
H(12B)	9397	2778	628	45
H(12C)	9831	2381	29	45
H(15)	9116	-989	-1626	44
H(16)	8997	-2913	-2463	53
H(17)	7952	-4871	-2600	55
H(18)	7063	-5020	-1870	51
H(19)	7199	-3139	-1017	43

Table 1. Crystal data and structure refinement for **14d**.

Identification code	**14d**	
Empirical formula	C14 H23 Al Cl4 N4 O2 Si	
Formula weight	476.23	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5697(11) Å	α= 94.449(3)°.
	b = 11.8936(16) Å	β= 107.249(3)°.
	c = 11.9049(15) Å	γ = 96.720(3)°.
Volume	1142.8(3) $Å^3$	
Z	2	
Density (calculated)	1.384 Mg/m^3	
Absorption coefficient	0.625 mm^{-1}	
F(000)	492	
Crystal size	0.4 x 0.4 x 0.2 mm^3	
Theta range for data collection	1.74 to 28.29°.	
Index ranges	-11<=h<=10, -15<=k<=15, -12<=l<=15	
Reflections collected	10229	
Independent reflections	5665 [R(int) = 0.0158]	
Completeness to theta = 28.29°	99.5 %	
Absorption correction	Empirical	
Max. and min. transmission	1 and 0.81	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5665 / 0 / 241	
Goodness-of-fit on F^2	1.047	

Final R indices [I>2sigma(I)]	R1 = 0.0476, wR2 = 0.1248
R indices (all data)	R1 = 0.0612, wR2 = 0.1340
Largest diff. peak and hole	0.840 and -0.788 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **14d**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Si(1)	1722(1)	2709(1)	7707(1)	24(1)
C(1)	-551(3)	3967(2)	7363(2)	36(1)
C(2)	-2018(3)	4335(2)	6538(3)	54(1)
C(3)	2547(3)	4676(2)	9522(2)	43(1)
C(4)	1088(3)	3003(2)	10004(2)	39(1)
C(5)	615(2)	1310(2)	7780(2)	27(1)
C(6)	-1079(2)	1029(2)	7194(2)	31(1)
C(7)	-1929(3)	-13(2)	7268(2)	39(1)
C(8)	-1096(3)	-793(2)	7913(2)	47(1)
C(9)	576(3)	-536(2)	8493(3)	48(1)
C(10)	1430(3)	509(2)	8436(2)	37(1)
C(11)	4704(3)	2381(2)	8022(2)	33(1)
C(12)	6321(3)	2208(2)	8829(2)	45(1)
C(13)	1625(4)	1391(3)	5495(2)	58(1)
C(14)	2851(4)	3368(3)	5733(3)	60(1)
N(1)	1292(2)	3635(1)	9015(2)	30(1)
N(2)	-270(2)	4059(2)	8476(2)	35(1)
N(3)	2595(2)	2369(2)	6383(2)	37(1)
N(4)	4241(2)	2061(2)	6916(2)	41(1)
O(1)	471(2)	3504(1)	6846(1)	34(1)
O(2)	3720(2)	2902(1)	8532(1)	31(1)
Al(1)	3734(1)	7575(1)	7179(1)	38(1)
Cl(1)	5262(1)	6299(1)	7169(1)	106(1)
Cl(2)	1386(1)	6772(1)	7188(1)	82(1)
Cl(3)	3486(2)	8428(1)	5662(1)	98(1)
Cl(4)	4903(1)	8776(1)	8699(1)	51(1)

Table 3. Bond lengths [Å] and angles [°] for **14d**.

Si(1)-O(2)	1.6806(15)	C(8)-C(9)	1.379(4)
Si(1)-O(1)	1.6822(15)	C(9)-C(10)	1.384(3)
Si(1)-C(5)	1.838(2)	C(11)-N(4)	1.271(3)
Si(1)-N(3)	1.9699(18)	C(11)-O(2)	1.353(2)
Si(1)-N(1)	1.9855(17)	C(11)-C(12)	1.481(3)
C(1)-N(2)	1.268(3)	C(13)-N(3)	1.491(3)
C(1)-O(1)	1.352(3)	C(14)-N(3)	1.497(3)
C(1)-C(2)	1.483(3)	N(1)-N(2)	1.468(2)
C(3)-N(1)	1.497(3)	N(3)-N(4)	1.468(3)
C(4)-N(1)	1.487(3)	Al(1)-Cl(3)	2.1090(11)
C(5)-C(10)	1.398(3)	Al(1)-Cl(1)	2.1185(11)
C(5)-C(6)	1.398(3)	Al(1)-Cl(4)	2.1227(9)
C(6)-C(7)	1.386(3)	Al(1)-Cl(2)	2.1274(11)
C(7)-C(8)	1.378(4)		

O(2)-Si(1)-O(1)	135.19(8)	C(9)-C(10)-C(5)	120.5(2)
O(2)-Si(1)-C(5)	112.96(8)	N(4)-C(11)-O(2)	121.0(2)
O(1)-Si(1)-C(5)	111.83(9)	N(4)-C(11)-C(12)	122.94(19)
O(2)-Si(1)-N(3)	84.07(8)	O(2)-C(11)-C(12)	116.02(19)
O(1)-Si(1)-N(3)	88.16(8)	N(2)-N(1)-C(4)	107.50(16)
C(5)-Si(1)-N(3)	101.74(8)	N(2)-N(1)-C(3)	105.56(16)
O(2)-Si(1)-N(1)	87.48(7)	C(4)-N(1)-C(3)	108.59(18)
O(1)-Si(1)-N(1)	83.52(7)	N(2)-N(1)-Si(1)	105.64(12)
C(5)-Si(1)-N(1)	100.37(8)	C(4)-N(1)-Si(1)	115.25(13)
N(3)-Si(1)-N(1)	157.89(8)	C(3)-N(1)-Si(1)	113.64(13)
N(2)-C(1)-O(1)	121.59(19)	C(1)-N(2)-N(1)	108.44(16)
N(2)-C(1)-C(2)	123.0(2)	N(4)-N(3)-C(13)	106.86(19)
O(1)-C(1)-C(2)	115.4(2)	N(4)-N(3)-C(14)	105.89(19)
C(10)-C(5)-C(6)	118.28(18)	C(13)-N(3)-C(14)	108.2(2)
C(10)-C(5)-Si(1)	121.18(15)	N(4)-N(3)-Si(1)	105.98(13)
C(6)-C(5)-Si(1)	120.53(15)	C(13)-N(3)-Si(1)	115.15(15)
C(7)-C(6)-C(5)	120.8(2)	C(14)-N(3)-Si(1)	114.10(17)
C(8)-C(7)-C(6)	119.8(2)	C(11)-N(4)-N(3)	108.87(17)
C(7)-C(8)-C(9)	120.3(2)	C(1)-O(1)-Si(1)	113.96(14)
C(8)-C(9)-C(10)	120.3(2)	C(11)-O(2)-Si(1)	114.07(13)

Cl(3)-Al(1)-Cl(1)	109.64(7)	Cl(3)-Al(1)-Cl(2)	110.32(5)
Cl(3)-Al(1)-Cl(4)	108.31(5)	Cl(1)-Al(1)-Cl(2)	108.20(5)
Cl(1)-Al(1)-Cl(4)	108.16(4)	Cl(4)-Al(1)-Cl(2)	112.17(5)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **14d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si(1)	23(1)	24(1)	26(1)	2(1)	9(1)	3(1)
C(1)	31(1)	26(1)	48(1)	5(1)	9(1)	7(1)
C(2)	43(1)	50(2)	67(2)	16(1)	6(1)	21(1)
C(3)	33(1)	35(1)	55(2)	-16(1)	12(1)	-1(1)
C(4)	35(1)	54(1)	31(1)	1(1)	14(1)	9(1)
C(5)	27(1)	26(1)	27(1)	2(1)	10(1)	3(1)
C(6)	29(1)	32(1)	30(1)	2(1)	7(1)	3(1)
C(7)	32(1)	42(1)	41(1)	-2(1)	11(1)	-6(1)
C(8)	50(1)	34(1)	59(2)	7(1)	23(1)	-6(1)
C(9)	48(1)	36(1)	62(2)	21(1)	15(1)	9(1)
C(10)	30(1)	33(1)	46(1)	11(1)	7(1)	6(1)
C(11)	28(1)	30(1)	47(1)	2(1)	20(1)	3(1)
C(12)	26(1)	54(1)	60(2)	2(1)	18(1)	10(1)
C(13)	61(2)	74(2)	37(1)	-16(1)	19(1)	2(1)
C(14)	67(2)	76(2)	54(2)	33(2)	35(2)	15(2)
N(1)	22(1)	32(1)	34(1)	-3(1)	8(1)	5(1)
N(2)	25(1)	33(1)	47(1)	-1(1)	10(1)	9(1)
N(3)	40(1)	44(1)	31(1)	5(1)	17(1)	7(1)
N(4)	39(1)	48(1)	45(1)	4(1)	24(1)	11(1)
O(1)	37(1)	32(1)	33(1)	8(1)	8(1)	10(1)
O(2)	23(1)	35(1)	36(1)	-4(1)	11(1)	4(1)
Al(1)	32(1)	37(1)	39(1)	4(1)	3(1)	5(1)
Cl(1)	65(1)	79(1)	142(1)	-43(1)	-12(1)	39(1)
Cl(2)	50(1)	59(1)	130(1)	9(1)	28(1)	-13(1)
Cl(3)	116(1)	102(1)	41(1)	24(1)	-14(1)	-32(1)
Cl(4)	46(1)	64(1)	39(1)	-8(1)	10(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **14d**.

	x	y	z	U(eq)
H(2A)	-2657	4685	6993	81
H(2B)	-2708	3672	6010	81
H(2C)	-1658	4892	6067	81
H(3A)	2760	5068	8877	65
H(3B)	3575	4453	10011	65
H(3C)	2126	5189	10011	65
H(4A)	814	3514	10581	59
H(4B)	2120	2719	10391	59
H(4C)	196	2358	9692	59
H(6)	-1654	1560	6740	37
H(7)	-3083	-190	6876	47
H(8)	-1677	-1510	7959	56
H(9)	1143	-1078	8934	58
H(10)	2579	683	8846	44
H(12A)	6901	1781	8384	68
H(12B)	6145	1778	9462	68
H(12C)	6985	2950	9176	68
H(13A)	2162	1274	4882	87
H(13B)	504	1555	5129	87
H(13C)	1573	700	5889	87
H(14A)	3437	4033	6304	90
H(14B)	1777	3539	5258	90
H(14C)	3506	3188	5211	90