SUPPLEMENTARY MATERIAL

DONOR-ACCEPTOR INTERACTIONS IN CRYSTAL ENGINEERING

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Table 1. Crystal Data and Structure Refinement for $C_{31}H_{26}F_6N_2O_6S_2$.

Empirical formula	$C_{31}H_{26}F_6N_2O_6S_2$
Formula weight	700.66
Temperature	173(2) K
Wavelength	0.71070 A
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	a = 11.3671(9) A α = 90 deg.
	b = 22.1802(18) A β = 90 deg.
	c = 25.876(2) A γ = 90 deg.
Volume	6524.0(9) A^3
Z, Calculated density	8, 1.427 Mg/m^3
Absorption coefficient	0.243 mm^{-1}
F(000)	2880
Crystal size	0.40 x 0.35 x 0.20 mm
Theta range for data collection	1.57 to 24.71 deg.
Limiting indices	-13<=h<=13, -23<=k<=26, -30<=l<=27
Reflections collected / unique	32194 / 5565 [R(int) = 0.1031]
Completeness to theta = 24.71	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9530 and 0.9091
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5565 / 0 / 427

Goodness-of-fit on F^2	1.032
Final R indices [I>2sigma(I)]	R1 = 0.0616, wR2 = 0.1431
R indices (all data)	R1 = 0.1080, wR2 = 0.1659
Largest diff. peak and hole	0.791 and -0.295 $e.A^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for $C_{31}H_{26}F_6N_2O_6S_2$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	8166(1)	114(1)	5801(1)	36(1)
S(2)	13038(1)	2587(1)	5741(1)	34(1)
N(1)	7171(3)	2257(1)	5686(1)	31(1)
N(2)	12804(3)	5440(1)	5572(1)	33(1)
C(12)	10826(3)	5120(2)	5607(1)	35(1)
O(4)	13502(3)	1989(1)	5735(1)	57(1)
C(6)	9624(3)	3655(2)	5598(1)	36(1)
C(1)	6788(3)	2831(2)	5702(1)	37(1)
C(7)	10342(3)	4047(2)	5585(1)	36(1)
O(5)	13899(2)	3048(1)	5681(1)	56(1)
C(4)	9141(3)	2582(2)	5606(1)	34(1)
C(3)	8759(3)	3178(2)	5624(1)	32(1)
C(8)	11191(3)	4518(2)	5578(1)	31(1)
F(5)	11682(3)	2287(1)	6510(1)	86(1)
C(13)	6311(3)	1761(2)	5692(2)	46(1)
C(11)	11656(3)	5573(2)	5604(1)	36(1)

C(10)	13176(3)	4862(2)	5546(1)	36(1)
C(2)	7578(3)	3300(2)	5671(1)	38(1)
C(5)	8317(3)	2134(2)	5638(1)	35(1)
O(2)	8566(3)	720(1)	5771(1)	75(1)
O(6)	11991(2)	2675(2)	5446(1)	60(1)
O(1)	8971(2)	-316(1)	5592(1)	53(1)
C(14)	13675(3)	5929(2)	5565(2)	48(1)
C(9)	12389(3)	4398(2)	5549(1)	36(1)
F(6)	12081(3)	3223(1)	6475(1)	93(1)
F(4)	13364(3)	2584(2)	6736(1)	107(1)
C(30)	8222(5)	-50(2)	6486(2)	58(1)
F(2)	7885(4)	-594(1)	6586(1)	111(1)
O(3)	6973(3)	12(2)	5666(1)	74(1)
F(1)	9276(4)	41(2)	6668(1)	143(2)
C(31)	12524(4)	2679(2)	6399(2)	54(1)
F(3)	7501(3)	310(2)	6747(1)	103(1)
C(22)	5017(4)	1122(2)	7017(2)	46(1)
C(17)	7803(4)	1849(2)	6990(2)	51(1)
C(15)	8270(4)	2910(2)	7036(2)	49(1)
C(23)	4114(4)	670(2)	6992(1)	45(1)
C(21)	5746(4)	1504(2)	7033(2)	46(1)
C(26)	2364(5)	-202(2)	6938(2)	63(1)
C(25)	3522(5)	-367(2)	6968(2)	62(1)

C(18)	6625(4)	1980(2)	7040(2)	45(1)
C(28)	2931(4)	836(2)	6964(2)	53(1)
C(19)	6263(4)	2576(2)	7089(2)	50(1)
C(20)	7082(4)	3035(2)	7087(2)	53(1)
C(16)	8624(4)	2316(2)	6987(2)	55(1)
C(24)	4399(4)	60(2)	6994(2)	53(1)
C(27)	2061(4)	403(2)	6937(2)	59(1)
C(29)	9165(5)	3409(2)	7040(2)	86(2)

Table 3. Bond lengths [A] and angles [deg] for $C_{31}H_{26}F_6N_2O_6S_2$.

S(1)-O(3)	1.418(3)	S(1)-O(2)	1.421(3)
S(1)-O(1)	1.429(3)	S(1)-C(30)	1.810(5)
S(2)-O(5)	1.424(3)	S(2)-O(4)	1.427(3)
S(2)-O(6)	1.428(3)	S(2)-C(31)	1.811(4)
N(1)-C(5)	1.337(4)	N(1)-C(1)	1.347(4)
N(1)-C(13)	1.471(4)	N(2)-C(11)	1.341(4)
N(2)-C(10)	1.350(4)	N(2)-C(14)	1.469(4)
C(12)-C(11)	1.379(5)	C(12)-C(8)	1.401(5)
C(6)-C(7)	1.193(5)	C(6)-C(3)	1.447(5)
C(1)-C(2)	1.377(5)	C(7)-C(8)	1.421(5)
C(4)-C(5)	1.369(5)	C(4)-C(3)	1.392(5)
C(3)-C(2)	1.374(5)	C(8)-C(9)	1.390(5)
F(5)-C(31)	1.325(5)	C(10)-C(9)	1.365(5)
F(6)-C(31)	1.322(5)	F(4)-C(31)	1.310(5)
C(30)-F(2)	1.292(5)	C(30)-F(1)	1.302(6)
C(30)-F(3)	1.328(5)	C(22)-C(21)	1.186(5)
C(22)-C(23)	1.437(6)	C(17)-C(18)	1.376(6)
C(17)-C(16)	1.394(6)	C(15)-C(16)	1.384(6)
C(15)-C(20)	1.385(6)	C(15)-C(29)	1.505(6)
C(23)-C(24)	1.390(5)	C(23)-C(28)	1.396(6)
C(21)-C(18)	1.454(6)	C(26)-C(25)	1.369(7)

C(26)-C(27)	1.387(6)	C(25)-C(24)	1.378(6)
C(18)-C(19)	1.390(5)	C(28)-C(27)	1.380(6)
C(19)-C(20)	1.378(6)		

O(3)-S(1)-O(2)	116.3(2)	O(3)-S(1)-O(1)	114.4(2)
O(2)-S(1)-O(1)	113.87(19)	O(3)-S(1)-C(30)	104.0(2)
O(2)-S(1)-C(30)	103.5(2)	O(1)-S(1)-C(30)	102.5(2)
O(5)-S(2)-O(4)	114.36(18)	O(5)-S(2)-O(6)	114.63(19)
O(4)-S(2)-O(6)	115.42(19)	O(5)-S(2)-C(31)	104.0(2)
O(4)-S(2)-C(31)	103.58(19)	O(6)-S(2)-C(31)	102.59(19)
C(5)-N(1)-C(1)	120.7(3)	C(5)-N(1)-C(13)	119.8(3)
C(1)-N(1)-C(13)	119.5(3)	C(11)-N(2)-C(10)	121.2(3)
C(11)-N(2)-C(14)	119.6(3)	C(10)-N(2)-C(14)	119.3(3)
C(11)-C(12)-C(8)	119.5(3)	C(7)-C(6)-C(3)	178.8(4)
N(1)-C(1)-C(2)	120.2(3)	C(6)-C(7)-C(8)	179.0(4)
C(5)-C(4)-C(3)	118.3(3)	C(2)-C(3)-C(4)	119.7(3)
C(2)-C(3)-C(6)	121.6(3)	C(4)-C(3)-C(6)	118.7(3)
C(9)-C(8)-C(12)	118.4(3)	C(9)-C(8)-C(7)	121.7(3)
C(12)-C(8)-C(7)	119.9(3)	N(2)-C(11)-C(12)	120.4(3)
N(2)-C(10)-C(9)	120.7(3)	C(1)-C(2)-C(3)	119.5(3)
N(1)-C(5)-C(4)	121.6(3)	C(10)-C(9)-C(8)	119.9(3)
F(2)-C(30)-F(1)	110.2(5)	F(2)-C(30)-F(3)	106.0(4)
F(1)-C(30)-F(3)	106.9(4)	F(2)-C(30)-S(1)	111.9(3)

F(1)-C(30)-S(1)	110.8(4)	F(3)-C(30)-S(1)	110.8(4)
F(4)-C(31)-F(6)	109.0(4)	F(4)-C(31)-F(5)	106.0(4)
F(6)-C(31)-F(5)	106.9(4)	F(4)-C(31)-S(2)	111.9(3)
F(6)-C(31)-S(2)	111.5(3)	F(5)-C(31)-S(2)	111.3(3)
C(21)-C(22)-C(23)	178.6(5)	C(18)-C(17)-C(16)	119.7(4)
C(16)-C(15)-C(20)	118.9(4)	C(16)-C(15)-C(29)	120.3(4)
C(20)-C(15)-C(29)	120.8(4)	C(24)-C(23)-C(28)	118.9(4)
C(24)-C(23)-C(22)	120.8(4)	C(28)-C(23)-C(22)	120.3(4)
C(22)-C(21)-C(18)	178.3(5)	C(25)-C(26)-C(27)	119.8(5)
C(26)-C(25)-C(24)	121.0(4)	C(17)-C(18)-C(19)	119.9(4)
C(17)-C(18)-C(21)	120.9(4)	C(19)-C(18)-C(21)	119.3(4)
C(27)-C(28)-C(23)	120.5(4)	C(20)-C(19)-C(18)	120.1(4)
C(19)-C(20)-C(15)	120.8(4)	C(15)-C(16)-C(17)	120.8(4)
C(25)-C(24)-C(23)	120.0(4)	C(28)-C(27)-C(26)	119.8(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($A^2 \times 10^3$) for $C_{31}H_{26}F_6N_2O_6S_2$. The anisotropic displacement factor exponent takes the form:

$$-2\,pi^2\,[\,h^2\,a^{*2}\,U11 + \ldots + 2\,h\,k\,a^*\,b^*\,U12]$$

	U11	U22	U33	U23	U13	U12
S(1)	31(1)	30(1)	47(1)	6(1)	0(1)	-1(1)
S(2)	33(1)	30(1)	39(1)	-3(1)	-1(1)	5(1)
N(1)	33(2)	29(2)	32(2)	2(1)	-3(1)	-4(1)
N(2)	30(2)	31(2)	40(2)	-2(1)	-4(1)	-2(1)
C(12)	28(2)	32(2)	45(2)	-1(2)	0(2)	0(2)
O(4)	57(2)	28(2)	87(2)	-6(1)	15(2)	11(1)
C(6)	41(2)	29(2)	38(2)	-1(2)	-1(2)	1(2)
C(1)	33(2)	42(2)	37(2)	-6(2)	2(2)	8(2)
C(7)	42(2)	28(2)	38(2)	-2(2)	2(2)	0(2)
O(5)	49(2)	36(2)	82(2)	-3(1)	7(2)	-7(1)
C(4)	31(2)	32(2)	40(2)	4(2)	-1(2)	-1(2)
C(3)	42(2)	25(2)	29(2)	0(2)	3(2)	0(2)
C(8)	38(2)	25(2)	31(2)	1(2)	-1(2)	0(2)
F(5)	88(2)	94(2)	77(2)	25(2)	34(2)	10(2)
C(13)	42(2)	45(2)	52(3)	-3(2)	1(2)	-14(2)
C(11)	36(2)	25(2)	46(2)	-4(2)	1(2)	0(2)
C(10)	33(2)	37(2)	38(2)	2(2)	0(2)	6(2)

C(2)	45(2)	27(2)	42(2)	-3(2)	7(2)	6(2)
C(5)	39(2)	22(2)	44(2)	3(2)	-4(2)	0(2)
O(2)	85(2)	28(2)	112(3)	15(2)	26(2)	-10(2)
O(6)	42(2)	97(2)	40(2)	1(2)	-4(1)	11(2)
O(1)	51(2)	47(2)	63(2)	-8(1)	10(1)	7(1)
C(14)	37(2)	40(2)	68(3)	-8(2)	-1(2)	-11(2)
C(9)	44(2)	26(2)	37(2)	3(2)	-1(2)	9(2)
F(6)	136(3)	73(2)	71(2)	-24(2)	23(2)	42(2)
F(4)	105(3)	169(3)	47(2)	-5(2)	-29(2)	40(2)
C(30)	71(3)	58(3)	45(3)	-9(2)	0(2)	-4(3)
F(2)	206(4)	54(2)	73(2)	26(2)	27(2)	-9(2)
O(3)	33(2)	113(3)	75(2)	10(2)	-10(2)	-6(2)
F(1)	104(3)	252(5)	72(2)	4(3)	-45(2)	-33(3)
C(31)	60(3)	58(3)	45(3)	-1(2)	-4(2)	14(2)
F(3)	138(3)	90(2)	81(2)	-30(2)	48(2)	-7(2)
C(22)	56(3)	42(2)	41(2)	3(2)	2(2)	1(2)
C(17)	65(3)	42(2)	45(2)	-3(2)	2(2)	-2(2)
C(15)	62(3)	47(3)	38(2)	8(2)	-2(2)	-16(2)
C(23)	60(3)	42(2)	32(2)	1(2)	-1(2)	-7(2)
C(21)	54(3)	42(2)	41(2)	2(2)	3(2)	-2(2)
C(26)	72(4)	65(3)	51(3)	-3(2)	2(2)	-19(3)
C(25)	89(4)	40(2)	56(3)	-3(2)	-3(3)	-10(3)
C(18)	52(3)	45(2)	36(2)	4(2)	1(2)	-5(2)

C(28)	62(3)	50(3)	46(2)	0(2)	-3(2)	-1(2)
C(19)	54(3)	48(3)	48(3)	8(2)	3(2)	-3(2)
C(20)	63(3)	44(3)	53(3)	11(2)	1(2)	-3(2)
C(16)	53(3)	67(3)	45(3)	0(2)	2(2)	0(2)
C(24)	61(3)	44(3)	53(3)	-2(2)	-1(2)	5(2)
C(27)	60(3)	63(3)	54(3)	-5(2)	-3(2)	-8(3)
C(29)	84(4)	90(4)	86(4)	16(3)	-3(3)	-19(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for $C_{31}H_{26}F_6N_2O_6S_2$.

	x	y	z	U(eq)
H(12)	10013	5216	5630	42
H(1)	5971	2489	5573	41
H(13A)	5615	1884	5889	69
H(13B)	6665	1405	5854	69
H(13C)	6080	1664	5336	69
H(11)	11414	5982	5624	43
H(10)	13995	4779	5526	43
H(2)	7310	3705	5683	45
H(5)	8566	1725	5625	42
H(14A)	14177	5899	5872	73
H(14B)	13268	6318	5566	73
H(14C)	14161	5896	5254	73
H(9)	12660	3993	5531	43
H(17)	8055	1442	6958	61
H(26)	1768	-502	6917	75
H(25)	3724	-783	6972	74
H(28)	2724	1251	6964	63

H(19)	5450	2668	7124	60
H(20)	6828	3441	7122	64
H(16)	9437	2225	6950	66
H(24)	5200	-62	7012	63
H(27)	1258	520	6919	71
H(29A)	8899	3737	6815	130
H(29B)	9921	3255	6915	130
H(29C)	9259	3561	7394	130

Table 6. Torsion angles [deg] for $C_{31}H_{26}F_6N_2O_6S_2$.

C(5)-N(1)-C(1)-C(2)	-0.3(5)
C(13)-N(1)-C(1)-C(2)	-176.8(3)
C(3)-C(6)-C(7)-C(8)	-43(41)
C(5)-C(4)-C(3)-C(2)	0.0(5)
C(5)-C(4)-C(3)-C(6)	179.2(3)
C(7)-C(6)-C(3)-C(2)	101(20)
C(7)-C(6)-C(3)-C(4)	-78(20)
C(11)-C(12)-C(8)-C(9)	0.3(5)
C(11)-C(12)-C(8)-C(7)	179.6(3)
C(6)-C(7)-C(8)-C(9)	121(29)
C(6)-C(7)-C(8)-C(12)	-58(29)
C(10)-N(2)-C(11)-C(12)	-0.5(5)
C(14)-N(2)-C(11)-C(12)	179.7(3)
C(8)-C(12)-C(11)-N(2)	0.1(5)
C(11)-N(2)-C(10)-C(9)	0.4(5)
C(14)-N(2)-C(10)-C(9)	-179.7(3)
N(1)-C(1)-C(2)-C(3)	0.0(5)
C(4)-C(3)-C(2)-C(1)	0.1(5)
C(6)-C(3)-C(2)-C(1)	-179.1(3)
C(1)-N(1)-C(5)-C(4)	0.4(5)

C(13)-N(1)-C(5)-C(4)	176.9(3)
C(3)-C(4)-C(5)-N(1)	-0.3(5)
N(2)-C(10)-C(9)-C(8)	0.0(5)
C(12)-C(8)-C(9)-C(10)	-0.4(5)
C(7)-C(8)-C(9)-C(10)	-179.6(3)
O(3)-S(1)-C(30)-F(2)	58.2(4)
O(2)-S(1)-C(30)-F(2)	-179.8(4)
O(1)-S(1)-C(30)-F(2)	-61.1(4)
O(3)-S(1)-C(30)-F(1)	-178.3(4)
O(2)-S(1)-C(30)-F(1)	-56.3(4)
O(1)-S(1)-C(30)-F(1)	62.3(4)
O(3)-S(1)-C(30)-F(3)	-59.9(4)
O(2)-S(1)-C(30)-F(3)	62.1(4)
O(1)-S(1)-C(30)-F(3)	-179.3(3)
O(5)-S(2)-C(31)-F(4)	-63.4(4)
O(4)-S(2)-C(31)-F(4)	56.4(4)
O(6)-S(2)-C(31)-F(4)	176.8(3)
O(5)-S(2)-C(31)-F(6)	58.9(4)
O(4)-S(2)-C(31)-F(6)	178.7(3)
O(6)-S(2)-C(31)-F(6)	-60.8(4)
O(5)-S(2)-C(31)-F(5)	178.2(3)
O(4)-S(2)-C(31)-F(5)	-62.0(3)
O(6)-S(2)-C(31)-F(5)	58.4(3)

C(21)-C(22)-C(23)-C(24)	160(100)
C(21)-C(22)-C(23)-C(28)	-20(20)
C(23)-C(22)-C(21)-C(18)	-32(31)
C(27)-C(26)-C(25)-C(24)	-0.7(7)
C(16)-C(17)-C(18)-C(19)	-0.3(6)
C(16)-C(17)-C(18)-C(21)	178.7(4)
C(22)-C(21)-C(18)-C(17)	-119(17)
C(22)-C(21)-C(18)-C(19)	60(17)
C(24)-C(23)-C(28)-C(27)	-0.2(6)
C(22)-C(23)-C(28)-C(27)	179.6(4)
C(17)-C(18)-C(19)-C(20)	0.1(6)
C(21)-C(18)-C(19)-C(20)	-178.9(4)
C(18)-C(19)-C(20)-C(15)	0.1(6)
C(16)-C(15)-C(20)-C(19)	-0.1(6)
C(29)-C(15)-C(20)-C(19)	-179.3(4)
C(20)-C(15)-C(16)-C(17)	-0.1(6)
C(29)-C(15)-C(16)-C(17)	179.1(4)
C(18)-C(17)-C(16)-C(15)	0.3(6)
C(26)-C(25)-C(24)-C(23)	0.5(7)
C(28)-C(23)-C(24)-C(25)	-0.1(6)
C(22)-C(23)-C(24)-C(25)	-179.8(4)
C(23)-C(28)-C(27)-C(26)	0.0(7)
C(25)-C(26)-C(27)-C(28)	0.4(7)