Single Crystal X-ray Structural Features of Aromatic Compounds Having a Pentafluorosulfuranyl (SF_5) Functional Group

Junyi Du,[a] Guoxiong Hua,[a] Petr Beier,[b] Alexandra M. Z. Slawin and J. Derek Woollins*[a]

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Table S1. Crystal Data and Refinement Parameters for Compounds **1**–**3**

Experimental details	**1**	**2**	**3**
Empirical formula	$C_7H_4F_5NS$	$C_7H_5F_5O_2S$	$C_6H_5F_5OS$
Formula weight	229.17	248.17	220.16
Crystal system	orthorhombic	monoclinic	triclinic
Lattice parameters	a = 9.0180(10) Å	a = 14.7940(3) Å	a = 8.9060(11) Å
	b = 13.1840(15) Å	b = 7.6423(10) Å	b = 9.9670(13) Å
	c = 6.8640(8) Å	c = 15.8920(3) Å	c = 10.2890(14) Å
			α = 85.0500(5)°
		β = 100.5590(7)°	β = 83.2100(5)°
			γ = 66.3000(3)°
Volume (Å^3)	816.2(16)	1766.3(5)	829.7(19)
Space group	*Cmcm*	*P2$_1$/c*	*P-1*
Z value	4	8	4
Dcalc (g/cm^3)	1.865	1.866	1.762
No. of reflections measured (Total)	5302	14817	7169
Unique	810	3101	2925
R_{int}	0.0338	0.1008	0.0532
Residuals: R_1 (I>2.00σ(I))	0.0385	0.0477	0.0447
Residuals: wR_2 (all reflections)	0.0984	0.1048	0.1245

Table S2. Crystal Data and Refinement Parameters for Compounds **4**–**6**

Experimental details	**4**	**5**	**6**
Empirical formula	$C_{10}H_9F_5N_2S$	$C_6H_6F_5NOS$	$C_{20}H_{13}F_5N_2S$
Formula weight	284.25	235.17	408.39
Crystal system	monoclinic	trigonal	monoclinic
Lattice parameters	a = 5.8557(10) Å	a = 19.2690(4) Å	a = 14.6300(4) Å
	b = 23.7060(4) Å		b = 8.4764(18) Å
	c = 7.8738(14) Å	c = 11.9530(4) Å	c = 15.1300(3) Å
	β = 92.9630(10)°		β = 105.6450(9)°
Volume (Å^3)	1091.5(3)	3843.5(19)	1806.7(7)
Space group	*P2$_1$/n*	*R-3*	*P2$_1$/c*
Z value	4	18	4
Dcalc (g/cm^3)	1.730	1.829	1.501
No. of reflections measured (Total)	9398	11037	15091
Unique	1921	1496	3163
R_{int}	0.1367	0.1326	0.0735
Residuals: R_1 (I>2.00σ(I))	0.0637	0.0788	0.0585
Residuals: wR_2 (all reflections)	0.1803	0.1370	0.1243

Table S3. Crystal Data and Refinement Parameters for Compounds **7**–**9**

Experimental details	**7**	**8**	**9**
Empirical formula	$C_{10}H_8F_5NO_4S$	$C_{13}H_8F_5NOS$	$C_9H_7ClF_5NO_4S$
Formula weight	333.23	321.26	355.66
Crystal system	monoclinic	triclinic	triclinic
Lattice parameters	a = 5.6660(12) Å	a = 9.4750(4) Å	a = 5.2263(12) Å
	b = 24.9400(5) Å	b = 10.2960(5) Å	b = 8.7375(12) Å
	c = 9.9600(2) Å	c = 13.0060(6) Å	c = 14.6190(2) Å
		α = 88.8000(2)°	α = 78.3600(2)°
	β = 97.7200(3)°	β = 83.6700(2)°	β = 84.8500(2)°
		γ = 80.8580(19)°	γ = 86.9900(2)°
Volume (Å^3)	1396.0(5)	1245.1(10)	650.8(2)
Space group	*P2$_1$/c*	*P-1*	*P-1*
Z value	4	4	2
Dcalc (g/cm^3)	1.586	1.714	1.815
No. of reflections measured (Total)	11333	9572	5703
Unique	2453	4352	2285
R_{int}	0.2357	0.0814	0.1118
Residuals: R_1 (I>2.00σ(I))	0.1365	0.0514	0.0571
Residuals: wR_2 (all reflections)	0.2026	0.1227	0.1498

Table S4. Selected Bond Distances (Å) and Bond Angles (°) for Compounds **1**–**3**

	1	**2**	**3**
S(1)-F(5)*	1.588(2)	1.573(3)[1.579(3)]	1.607(3)[1.603(3)]
S(1)-C(1)	1.798(3)	1.795(4)[1.796(4)]	1.822(4)[1.823(4)]
S(1)-F(1)	1.582(2)	1.572(3)[1.579(3)]	1.590(3)[1.602(3)]
S(1)-F(2)	1.582(2)	1.585(3)[1.578(3)]	1.593(3)[1.598(3)]
S(1)-F(3)	1.582(2)	1.590(3)[1.574(3)]	1.604(3)[1.595(3)]
S(1)-F(4)	1.582(2)	1.577(3)[1.575(3)]	1.604(3)[1.607(3)]
C(1)-S(1)-F(5)	180.00	179.53(19)[179.83(18)]	179.29(12)[179.74(12)]
F(5)-S(1)-F(1)	87.49(3)	87.25(14)[87.71(14)]	87.23(14)[87.66(14)]
F(5)-S(1)-F(2)	87.49(3)	87.64(14)[87.61(14)]	87.94(14)[87.68(14)]
F(5)-S(1)-F(3)	87.49(3)	87.28(14[87.46(14)]	87.71(14)[87.78(14)]
F(5)-S(1)-F(4)	87.49(3)	87.55(14)[87.83(14)]	87.26(13)[87.31(14)]
C(1)-S(1)-F(1)	92.51(3)	92.04(17)[92.42(16)]	92.97(15)[92.09(15)]
C(1)-S(1)-F(2)	92.51(3)	92.00(16)[92.50(17)]	92.73(14)[92.25(15)]
C(1)-S(1)-F(3)	92.51(3)	92.42(17)[92.41(16)]	92.08(15)[92.47(14)]
C(1)-S(1)-F(4)	92.51(3)	92.81(16)[92.06(17)]	92.06(15)[92.76(15)]
F-S(1)-F**	89.68(10)	88.25(14)[87.71(14)]	90.45(13)[90.37(14)]
	89.68(10)	87.64(14)[87.61(14)]	89.85(13)[89.35(14)]
	90.11(10)	87.28(14)[87.46(14)]	89.85(13)[90.03(14)]
	90.11(10)	87.55(14)[87.84(14)]	89.33(13)[89.85(14)]
F-S(1)-F***	174.98(5)	175.16(14)[175.17(15)]	174.92(14)[175.40(13)]
	174.98(5)	175.53(14)[175.44(15)]	175.17(13)[174.99(13)]

*F atom labelling in **1** is different from others; ** the angles between the adjacent F_{eq} atoms; ***the angles between the opposite F_{eq} atoms

Table S5. Selected Bond Distances (Å) and Bond Angles (°) for Compounds **4**–**6**

	4	**5**	**6**
S(1)-F(5)	1.581(3)	1.585(4)	1.597(2)
S(1)-C(1)	1.794(5)	1.801(6)	1.812(4)
S(1)-F(1)	1.572(3)	1.618(3)	1.5851(19)
S(1)-F(2)	1.573(4)	1.609(4)	1.5881(19)
S(1)-F(3)	1.576(3)	1.591(3)	1.5930(19)
S(1)-F(4)	1.575(4)	1.582(5)	1.5923(19)
C(1)-S(1)-F(5)	179.90(2)	179.10(2)	179.52(12)
F(5)-S(1)-F(1)	87.42(18)	86.58(18)	87.16(11)
F(5)-S(1)-F(2)	87.82(19)	86.90(2)	87.50(11)
F(5)-S(1)-F(3)	87.14(18)	88.18(19)	87.24(11)
F(5)-S(1)-F(4)	87.48(19)	88.00(3)	87.52(11)
C(1)-S(1)-F(1)	92.60(2)	92.60(2)	93.32(13)
C(1)-S(1)-F(2)	92.40(2)	92.70(3)	92.47(13)
C(1)-S(1)-F(3)	92.80(2)	92.60(2)	92.28(13)
C(1)-S(1)-F(4)	92.30(2)	92.40(3)	93.50(13)
F-S(1)-F*	90.90(2)	88.72(19)	89.75(10)
	89.50(2)	90.60(2)	90.12(10)
	89.70(2)	89.40(2)	90.11(10)
	90.40(2)	90.80(2)	89.54(10)
F-S(1)-F**	175.29(19)	174.50(2)	174.40(13)
	174.56(19)	174.90(2)	175.02(13)

*The angles between the adjacent F_{eq} atoms; **the angles between the opposite F_{eq} atoms

Table S6. Selected Bond Distances (Å) and Bond Angles (°) for Compounds **7**–**9**

	7	**8**	**9**
S(1)-F(5)	1.598(7)	1.585(3)[1.580(3))	1.568(4)
S(1)-C(1)	1.804(10)	1.800(4)[1.803(4)]	1.795(5)
S(1)-F(1)	1.587(7)	1.577(3)[1.582(2)]	1.572(4)
S(1)-F(2)	1.608(7)	1.574(2)[1.574(2)]	1.579(4)
S(1)-F(3)	1.587(6)	1.576(3)[1.587(2)]	1.582(4)
S(1)-F(4)	1.603(7)	1.583(2)[1.574(3)]	1.579(4)
C(1)-S(1)-F(5)	179.70(4)	178.94(14)[179.45(16)]	179.60(2)
F(5)-S(1)-F(1)	88.40(3)	88.06(14)[88.13(13)]	88.00(2)
F(5)-S(1)-F(2)	88.20(3)	88.03(13)[87.15(13)]	88.30(2)
F(5)-S(1)-F(3)	87.80(3)	87.42(13)[87.68(13)]	88.00(2)
F(5)-S(1)-F(4)	87.70(3)	87.63(13)[87.47(13)]	88.01(2)
C(1)-S(1)-F(1)	91.90(4)	92.66(15)[92.35(14)]	92.20(2)
C(1)-S(1)-F(2)	91.70(4)	92.70(14)[92.60(15)]	91.30(2)
C(1)-S(1)-F(3)	92.00(4)	91.86(15)[91.83(15)]	91.80(2)
C(1)-S(1)-F(4)	92.40(4)	91.59(14)[92.78(15)]	92.40(2)
F-S(1)-F*	89.90(3)	89.59(14)[89.75(13)]	90.40(2)
	90.00(3)	89.96(15)[90.20(14)]	90.00(2)
	89.90(3)	90.06(13)[89.81(12)]	89.60(2)
	89.80(3)	90.05(14)[89.84(13)]	89.79(19)
F-S(1)-F**	175.90(4)	175.48(14)[175.81(14)]	176.00(2)
	176.20(4)	175.70(14)[174.61(14)]	176.30(2)

*The angles between the adjacent F_{eq} atoms; **the angles between the opposite F_{eq} atoms

Table S7. Selected Intramolecular or Intermolecular Interactions (Å) and Angles (°) for Compounds **4**–**9**

	4	**5**	**6**	**7**	**8**	**9**
Intramolecular interactions						
F(1)···H(2)	2.619(3)	2.499(4)	2.421(2)	2.597(8)	2.517(4)[2.645(4)]	2.471(3)
F(2)···H(2)	2.390(3)	2.533(3)	2.628(2)	2.554(8)	2.461(4)[2.385(4)]	2.520(3)
F(3)···H(6)	2.644(3)	2.538(4)	2.453(2)	2.528(8)	2.529(4)[2.643(4)]	2.491(4)
F(4)···H(6)	2.435(2)	2.552(4)	2.658(2)	2.521(8)	2.490(5)[2.415(4)]	2.503(3)
C_{aryl}-H···N	2.560(3) 2.583(3)	2.620(6)	2.599(3), 2.591(3)	2.572(13)	2.706(5)[2.701(5)]	2.557(5)
C_{phenyl}-H···N			2.687(2), 2.817(3)			
C_{aryl}-H···O		2.653(4)		2.342(9)	2.410(4)[2.402(4)]	2.464(4)
C_{alkyl}-H···O						2.227(5)
N-H···O		2.364(3)				
Intermolecular interactions						
C-H···N	2.744(3)					
O-H···N		2.063(5)				
C_{aryl}-H···N		2.977(4)	2.661(2), 2.715(3)		2.429(5)	
C_{aryl}-H···O		2.543(5)		2.645(8) 2.748(8)	2.917(4), 2.942(4)	2.737(4) 2.829(5)
C-H···F	2.834(3) 2.630(3) 2.638(2)	2.725(6)	2.793(2)	2.583(8) 2.744(7) 2.767(8)	2.482(3)	
N-H···F		2.429(3)				