

# Single Crystal X-ray Structural Features of Aromatic Compounds Having a Pentafluorosulfuranyl (SF<sub>5</sub>) Functional Group

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

Experimental details	<b>1</b>	<b>2</b>	<b>3</b>
Empirical formula	C <sub>7</sub> H <sub>4</sub> F <sub>5</sub> NS	C <sub>7</sub> H <sub>5</sub> F <sub>5</sub> O <sub>2</sub> S	C <sub>6</sub> H <sub>5</sub> F <sub>5</sub> OS
Formula weight	229.17	248.17	220.16
Crystal system	orthorhombic	monoclinic	triclinic
Lattice parameters	<i>a</i> = 9.0180(10) Å <i>b</i> = 13.1840(15) Å <i>c</i> = 6.8640(8) Å	<i>a</i> = 14.7940(3) Å <i>b</i> = 7.6423(10) Å <i>c</i> = 15.8920(3) Å	<i>a</i> = 8.9060(11) Å <i>b</i> = 9.9670(13) Å <i>c</i> = 10.2890(14) Å <i>α</i> = 85.0500(5)° <i>β</i> = 83.2100(5)° <i>γ</i> = 66.3000(3)°
Volume (Å <sup>3</sup> )	816.2(16)	1766.3(5)	829.7(19)
Space group	<i>Cmcm</i>	<i>P2<sub>1</sub>/c</i>	<i>P-1</i>
Z value	4	8	4
D <sub>calc</sub> (g/cm <sup>3</sup> )	1.865	1.866	1.762
No. of reflections measured (Total)	5302	14817	7169
Unique	810	3101	2925
<i>R</i> <sub>int</sub>	0.0338	0.1008	0.0532
Residuals: <i>R</i> <sub>1</sub> ( <i>I</i> > 2.00σ( <i>I</i> ))	0.0385	0.0477	0.0447
Residuals: <i>wR</i> <sub>2</sub> (all reflections)	0.0984	0.1048	0.1245

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

Experimental details	<b>4</b>	<b>5</b>	<b>6</b>
Empirical formula	C <sub>10</sub> H <sub>9</sub> F <sub>5</sub> N <sub>2</sub> S	C <sub>6</sub> H <sub>6</sub> F <sub>5</sub> NOS	C <sub>20</sub> H <sub>13</sub> F <sub>5</sub> N <sub>2</sub> S
Formula weight	284.25	235.17	408.39
Crystal system	monoclinic	trigonal	monoclinic
Lattice parameters	$a = 5.8557(10) \text{ \AA}$ $b = 23.7060(4) \text{ \AA}$ $c = 7.8738(14) \text{ \AA}$ $\beta = 92.9630(10)^\circ$	$a = 19.2690(4) \text{ \AA}$ $c = 11.9530(4) \text{ \AA}$	$a = 14.6300(4) \text{ \AA}$ $b = 8.4764(18) \text{ \AA}$ $c = 15.1300(3) \text{ \AA}$ $\beta = 105.6450(9)^\circ$
Volume ( $\text{\AA}^3$ )	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 ( $\text{g/cm}^3$ )	1.730	1.829	1.501
No. of reflections measured (Total)	9398	11037	15091
Unique	1921	1496	3163
$R_{\text{int}}$	0.1367	0.1326	0.0735
Residuals: $R_1$ ( $I > 2.00\sigma(I)$ )	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	<b>7</b>	<b>8</b>	<b>9</b>
Empirical formula	C <sub>10</sub> H <sub>8</sub> F <sub>5</sub> NO <sub>4</sub> S	C <sub>13</sub> H <sub>8</sub> F <sub>5</sub> NOS	C <sub>9</sub> H <sub>7</sub> ClF <sub>5</sub> NO <sub>4</sub> S
Formula weight	333.23	321.26	355.66
Crystal system	monoclinic	triclinic	triclinic
Lattice parameters	$a = 5.6660(12) \text{ \AA}$ $b = 24.9400(5) \text{ \AA}$ $c = 9.9600(2) \text{ \AA}$ $\beta = 97.7200(3)^\circ$	$a = 9.4750(4) \text{ \AA}$ $b = 10.2960(5) \text{ \AA}$ $c = 13.0060(6) \text{ \AA}$ $\alpha = 88.8000(2)^\circ$ $\beta = 83.6700(2)^\circ$ $\gamma = 80.8580(19)^\circ$	$a = 5.2263(12) \text{ \AA}$ $b = 8.7375(12) \text{ \AA}$ $c = 14.6190(2) \text{ \AA}$ $\alpha = 78.3600(2)^\circ$ $\beta = 84.8500(2)^\circ$ $\gamma = 86.9900(2)^\circ$
Volume ( $\text{\AA}^3$ )	1396.0(5)	1245.1(10)	650.8(2)
Space group	$P2_1/c$	$P-1$	$P-1$
Z value	4	4	2
Dcalc ( $\text{g/cm}^3$ )	1.586	1.714	1.815
No. of reflections measured (Total)	11333	9572	5703
Unique	2453	4352	2285
$R_{\text{int}}$	0.2357	0.0814	0.1118
Residuals: $R_1$ ( $I > 2.00\sigma(I)$ )	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**

	<b>1</b>	<b>2</b>	<b>3</b>
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<sub>eq</sub> atoms; \*\*\*the angles between the opposite F<sub>eq</sub> atoms

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

	<b>4</b>	<b>5</b>	<b>6</b>
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<sub>eq</sub> atoms; \*\*the angles between the opposite F<sub>eq</sub> atoms

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

	<b>7</b>	<b>8</b>	<b>9</b>
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<sub>eq</sub> atoms; \*\*the angles between the opposite F<sub>eq</sub> atoms

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

	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>	<b>8</b>	<b>9</b>
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 <sub>aryl</sub> -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 <sub>phenyl</sub> -H···N			2.687(2), 2.817(3)			
C <sub>aryl</sub> -H···O		2.653(4)		2.342(9)	2.410(4)[ 2.402(4)]	2.464(4)
C <sub>alkyl</sub> -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 <sub>aryl</sub> -H···N		2.977(4)	2.661(2), 2.715(3)		2.429(5)	
C <sub>aryl</sub> -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)				