

Supplementary Information Table 2 Crystallographic data for sulfones **5** to **7**, **9** to **12**, **15** and **16**.

Compound	5	6	7	9	10	11	12	15	R-16
Formula	C ₁₃ H ₁₀ F ₂ O ₂ S	C ₁₅ H ₁₆ O ₄ S	C ₁₃ H ₁₀ FNO ₄ S	C ₁₆ H ₁₈ O ₄ S	C ₁₄ H ₁₂ F ₂ O ₂ S	C ₁₄ H ₁₃ NO ₅ S	C ₁₄ H ₁₃ NO ₅ S	C ₁₄ H ₁₄ O ₂ S	C ₁₆ H ₁₈ O ₄ S
Formula Weight	268.27	292.34	295.28	306.36	282.30	307.31	307.31	246.31	306.36
T/K	100(2)	150(2)	120(2)	291(2)	100(2)	120(2)	123(2)	100(2)	180(2)
Crystal System	Orthorhombic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Orthorhombic	Monoclinic	Monoclinic	Monoclinic
Space Group	<i>Pca</i> 2 ₁	<i>Pc</i>	<i>Pc</i>	<i>Cc</i>	<i>Cc</i>	<i>P</i> 2 ₁ 2 ₁	<i>P</i> 2 ₁ / <i>c</i>	<i>Pn</i>	<i>P</i> 2 ₁
<i>a</i> /Å	8.7490(9)	15.345(14)	13.0726(6)	17.924(4)	16.3313(11)	5.13970(10)	13.691(3)	7.4697(8)	7.0952(3)
<i>b</i> /Å	5.3330(5)	5.395(2)	5.2890(2)	9.756(3)	19.8342(14)	10.62070(10)	12.8075(13)	5.6810(7)	12.2671(5)
<i>c</i> /Å	24.881(3)	8.604(7)	8.9303(3)	8.6720(17)	8.2586(5)	24.9841(5)	7.9667(10)	14.0467(16)	8.6368(4)
α /°	90	90	90	90	90	90	90	90	90
β /°	90	105.57(3)	90.231(3)	92.355(8)	109.308(2)	90	93.450(13)	91.800(2)	94.274(2)
γ /°	90	90	90	90	90	90	90	90	90
<i>V</i> /Å ³	1160.9(2)	686.2(9)	617.44(4)	1515.2(6)	2524.6(3)	1363.81(4)	1394.4(4)	595.78(12)	749.64(6)
<i>Z</i>	4	2	2	4	8	4	4	2	2
ρ_{calc} /gcm ⁻³	1.535	1.415	1.588	1.343	1.485	1.497	1.464	1.373	1.357
μ /mm ⁻¹	0.295	0.246	0.288	0.226	0.275	0.259	0.253	0.257	0.229
2 θ max/°	54.44	50.90	54.90	50.18	55.96	54.88	60.22	56.60	54.92
Total reflections	3939	2756	8984	7227	21292	17154	13717	6696	6258
Unique reflections	2355	2556	2674	2647	6027	3108	4067	2936	3212
Refls I>2 σ (I)	2144	1966	2607	1898	5865	2978	3598	2702	3052
<i>R</i> _{int}	0.0231	0.0359	0.0246	0.0547	0.0276	0.0298	0.0131	0.0368	0.0466
Parameters	163	183	181	193	345	191	203	155	193
<i>R</i> ₁ [F, I>2 σ (I)]	0.0296	0.0809	0.0263	0.0420	0.0249	0.0280	0.0294	0.0354	0.0319
<i>wR</i> ₂ (F ² , all data)	0.0718	0.2263	0.0675	0.0800	0.0670	0.0840	0.0836	0.0810	0.0810
Flack	0.05(7)	0.3(2)	-0.01(5)	0.07(7)	0.02(3)	-0.02(6)	-	0.003(63)	-0.08(6)
Hoofit ^a	0.10(4)	0.16(7)	-0.01(2)	0.09(6)	0.021(16)	-0.006(19)	-	0.03(5)	-0.07(3)

^a as implemented in PLATON