Supplementary Information

Silver Complex of an *N*-Heterocyclic Carbene Ligand with Bulky Thiocarbamate Groups

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Spectroscopic data

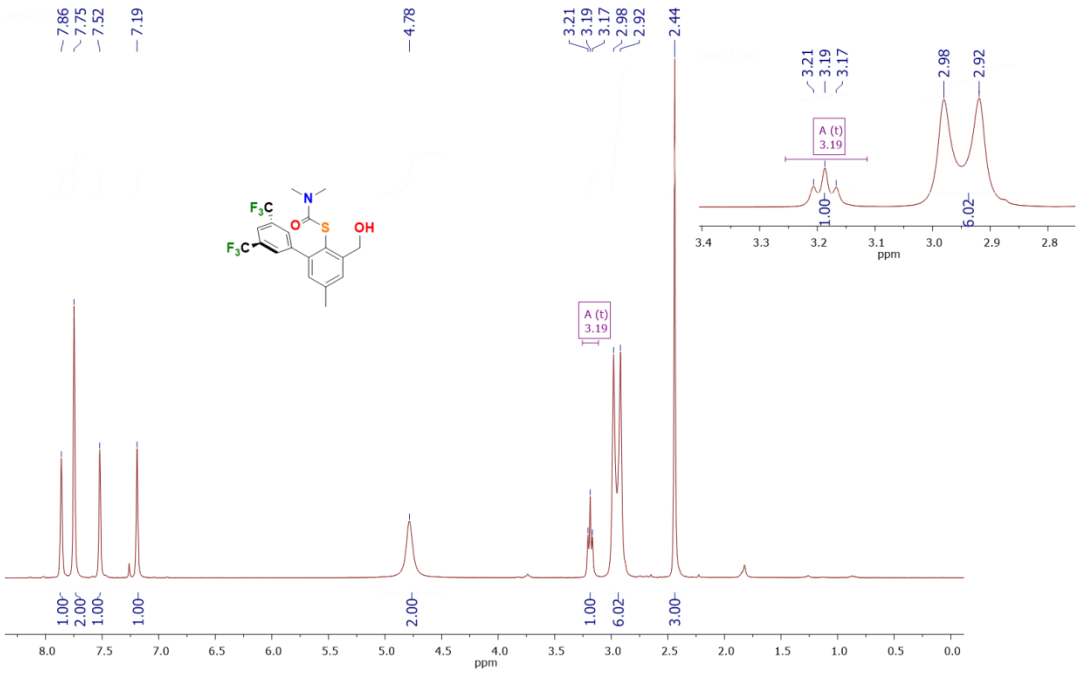

Figure S1. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **1**, inset: detail of resonances between 3.4-2.8 ppm.

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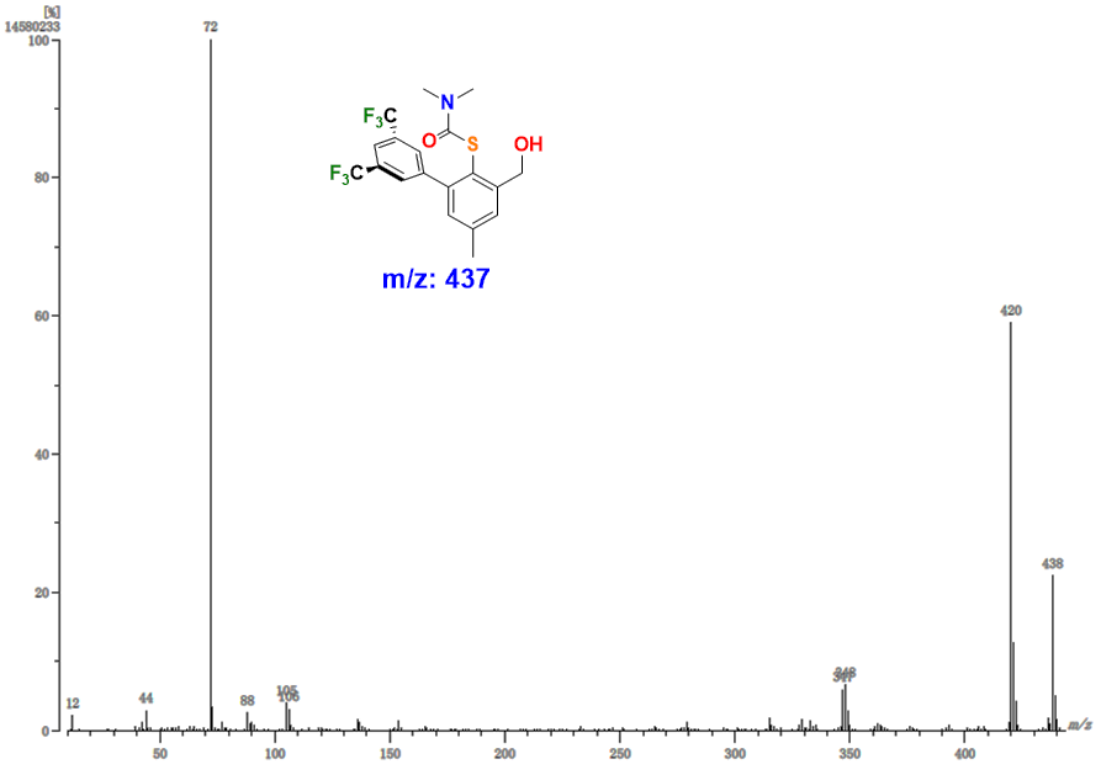

Figure S2. FAB$^+$ MS of **1** and its most important fragments.

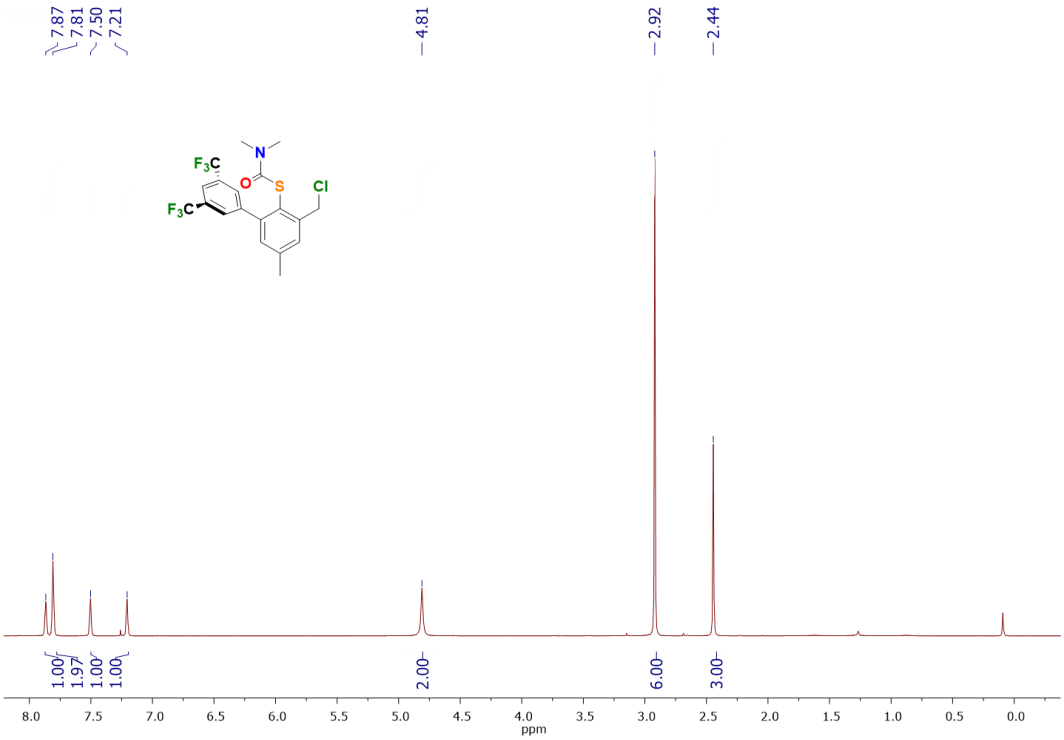

Figure S3. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of chloride **2** at room temperature.

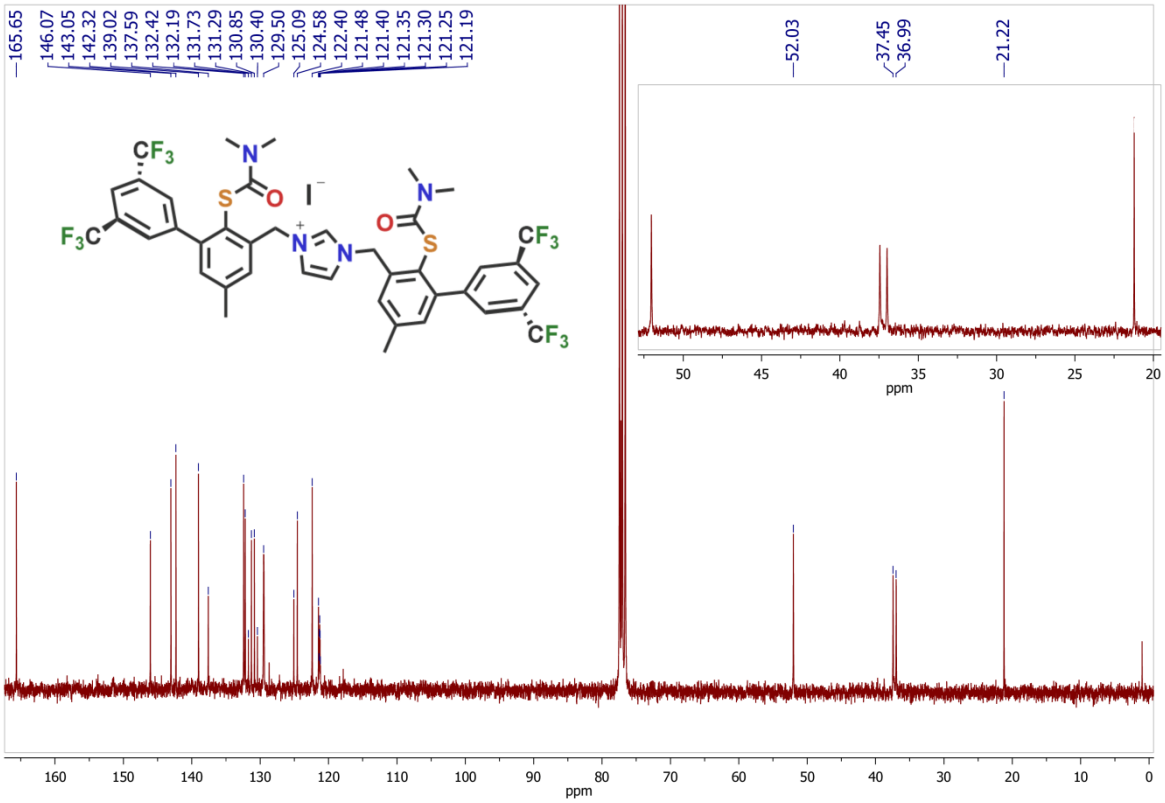

Figure S4. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of proligand **3** at room temperature.

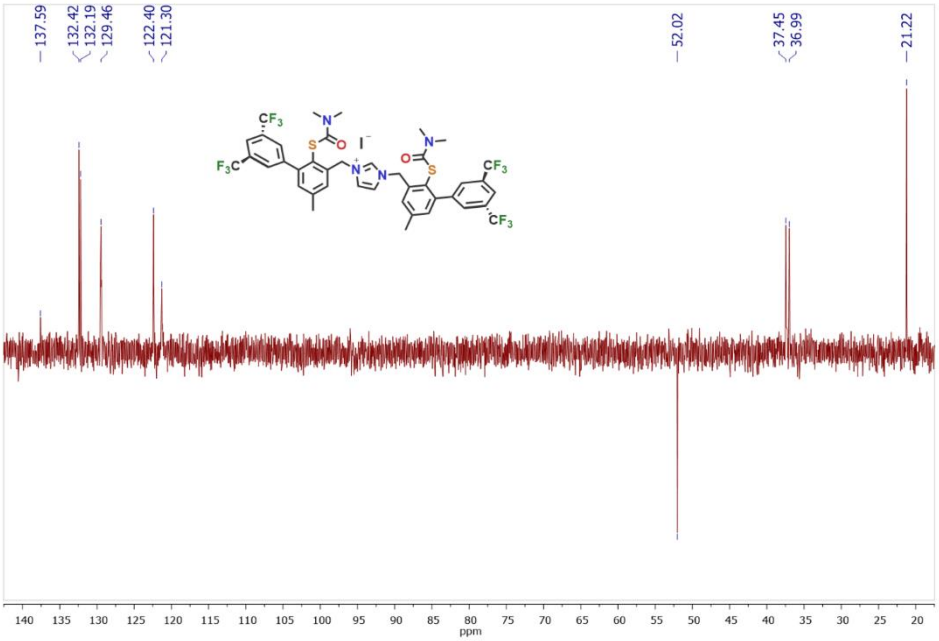

Figure S5. ^{13}C DEPT-135 NMR spectrum (75 MHz, $CDCl_3$) of proligand **3** at room temperature.

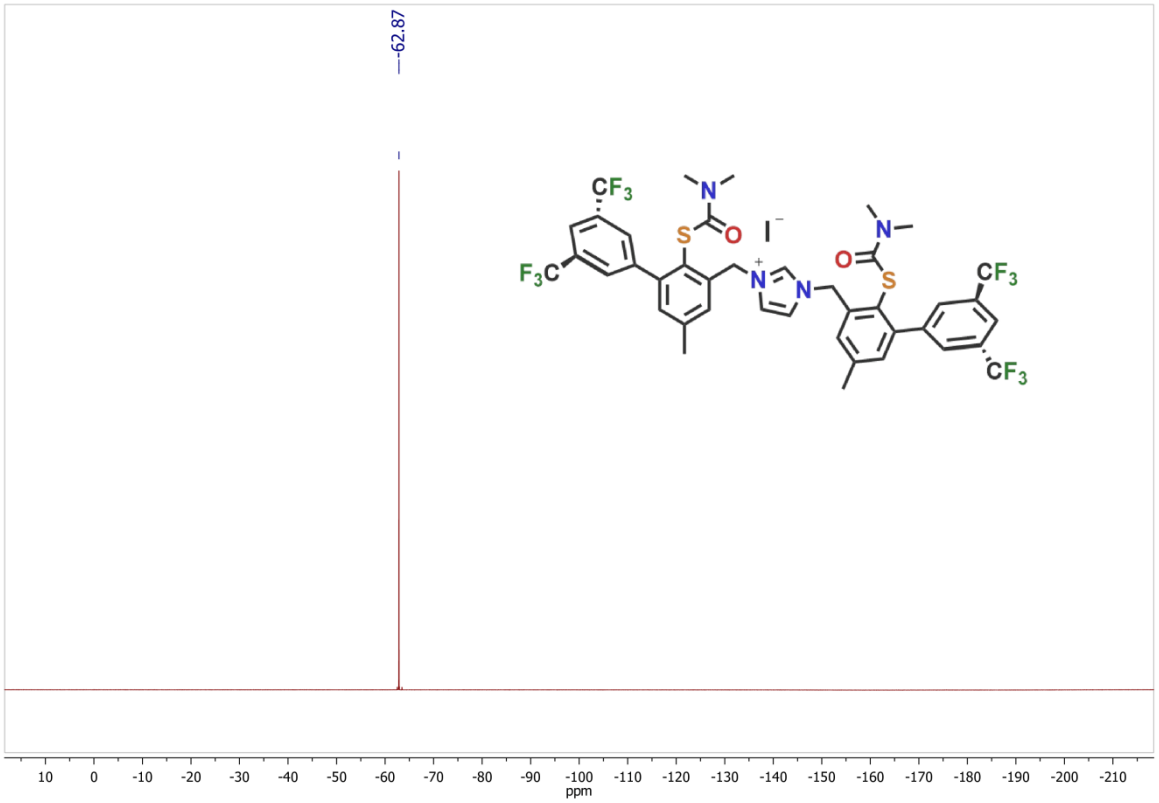

Figure S6. ^{19}F NMR spectrum (282 MHz, $CDCl_3$) of proligand **3** at room temperature.

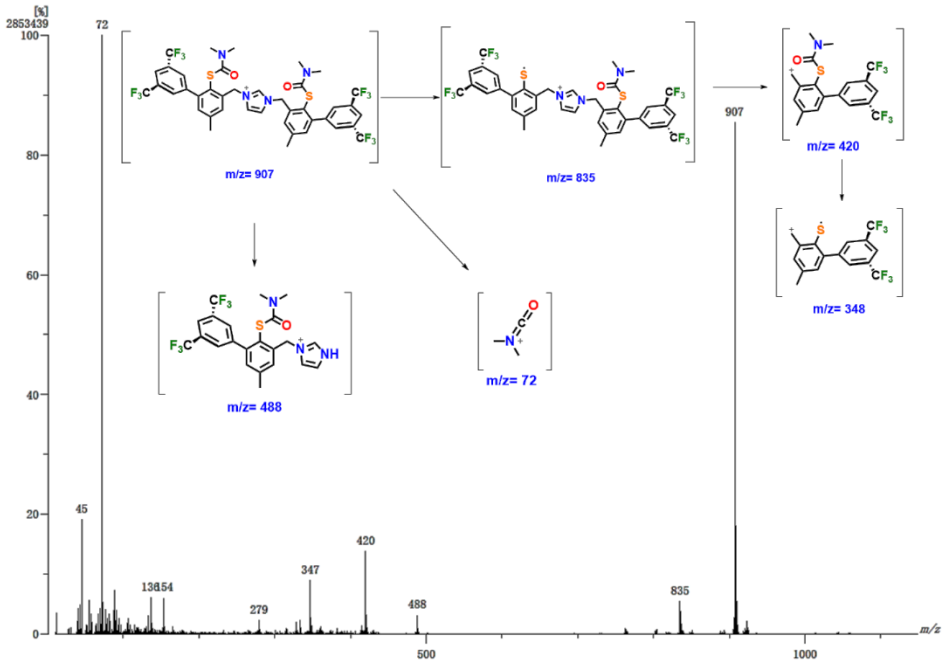

Figure S7. FAB$^+$ MS of **3** and its most important fragments.

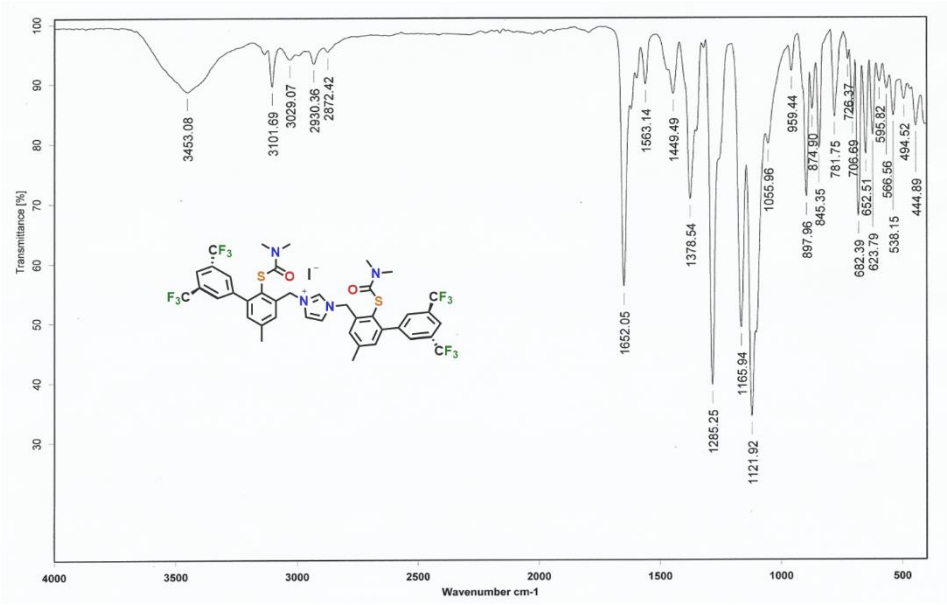

Figure S8. IR (KBr) spectrum of **3**.

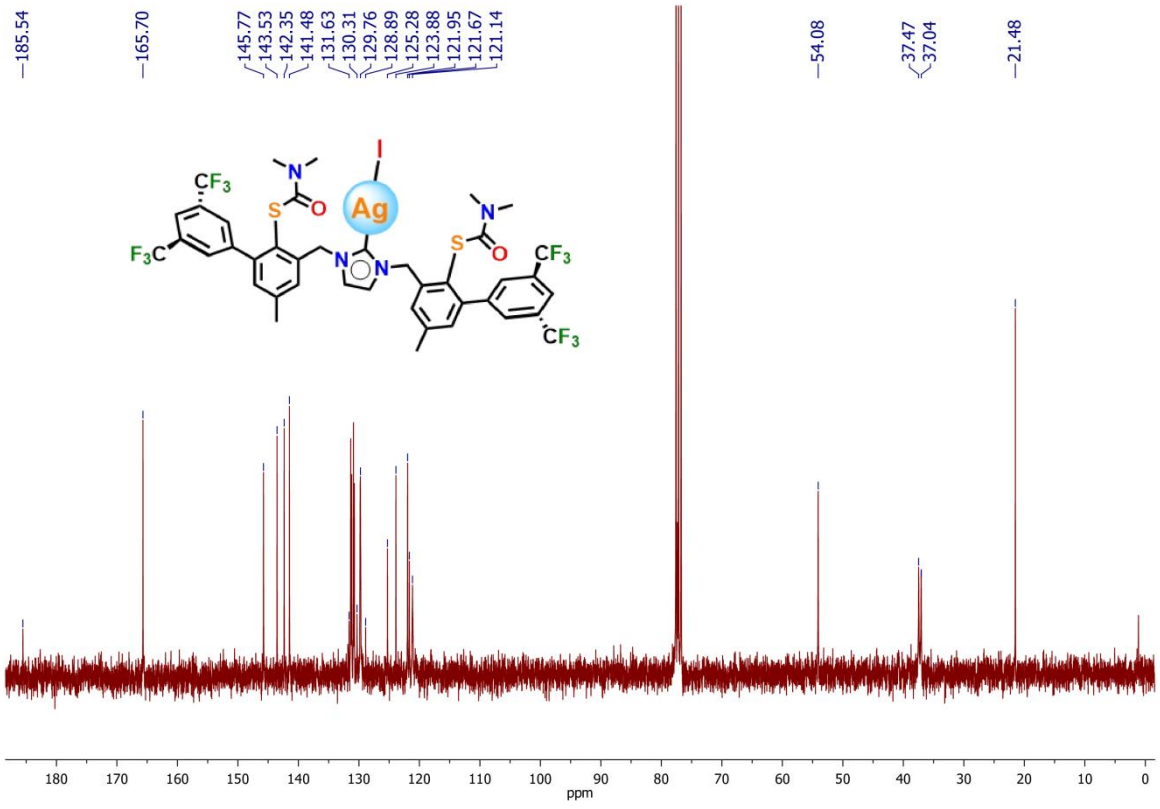

Figure S9. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of **5** at room temperature.

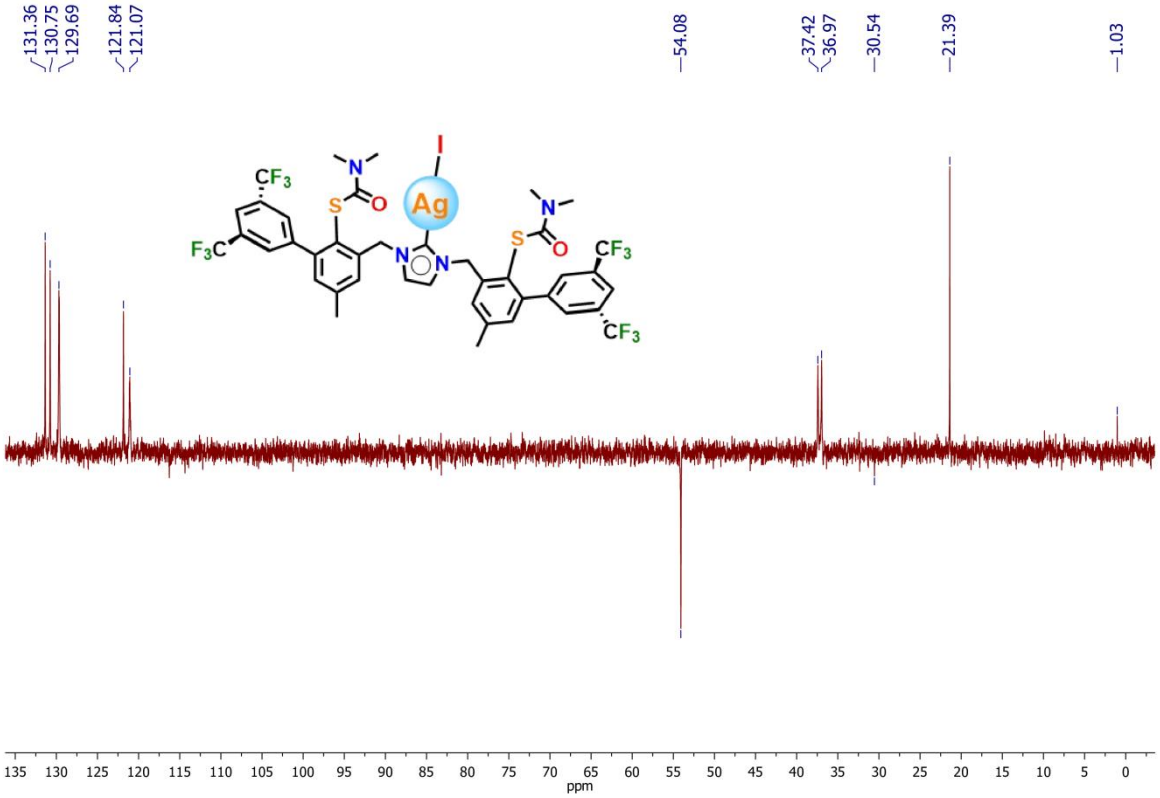

Figure S10. ^{13}C DEPT-135 NMR spectrum (75 MHz, $CDCl_3$) of **5** at room temperature.

Crystallographic data

Table S1. Crystal data and structure refinement for **1**

Identification code	**1**	
Empirical formula	$C_{19}H_{17}F_6NO_2S$	
Formula weight	437.40	
Temperature / K	130(2)	
Wavelength / Å	0.71073	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 5.134(2) Å	α = 99.45(2)°
	b = 10.620(4) Å	β = 96.43(3)°
	c = 17.878(4) Å	γ = 93.37(3)°
Volume / $Å^3$	952.6(6)	
Z	2	
Density (calculated) / (mg m^{-3})	1.525	
Absorption coefficient / mm^{-1}	0.242	
F(000)	448	
Crystal size / mm^3	0.54 × 0.07 × 0.06	
Theta range for data collection / degree	3.49-25.03	
Index ranges	$-6 \le h \le 6, -12 \le k \le 11, -21 \le l \le 20$	
Reflections collected	6227	
Independent reflections	3362 [R(int) = 0.0469]	
Completeness to theta = 25.03° / %	99.7	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	3362 / 1 / 268	
Goodness-of-fit on F^2	1.059	
Final R indices [I > 2sigma(I)]	R_1 = 0.0583, wR_2 = 0.1281	
R indices (all data)	R_1 = 0.0972, wR_2 = 0.1594	
Largest diff. peak and hole / $e.Å^{-3}$	0.340 and –0.344	

Table S2. Bond lengths and angles for **1**

Bond length / Å	
C(1)-C(2)	1.388(5)
C(1)-C(6)	1.391(5)
C(1)-C(9)	1.502(5)
C(2)-C(3)	1.393(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.390(5)
C(3)-C(7)	1.494(5)
C(4)-C(5)	1.387(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.385(5)
C(5)-C(8)	1.495(5)
C(6)-H(6)	0.9500
C(7)-F(3)	1.328(4)
C(7)-F(2)	1.336(5)
C(7)-F(1)	1.342(4)
C(8)-F(4)	1.325(5)
C(8)-F(6)	1.334(5)
C(8)-F(5)	1.336(5)
C(9)-C(10)	1.382(5)
C(9)-C(14)	1.408(5)
C(10)-C(11)	1.386(5)
C(10)-H(10)	0.9500
C(11)-C(12)	1.397(5)
C(11)-C(15)	1.496(5)
C(12)-C(13)	1.400(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.393(5)
C(13)-C(16)	1.514(5)
C(14)-S(1)	1.787(4)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-O(2)	1.432(4)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-O(1)	1.228(4)
C(17)-N(1)	1.346(4)
C(17)-S(1)	1.811(4)
C(18)-N(1)	1.471(5)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-N(1)	1.459(5)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
O(2)-H(2D)	0.876(19)
Bond angle / degree	
C(2)-C(1)-C(6)	118.9(3)
C(2)-C(1)-C(9)	119.7(3)
C(6)-C(1)-C(9)	121.5(3)
C(1)-C(2)-C(3)	120.8(3)
C(1)-C(2)-H(2)	119.6
C(3)-C(2)-H(2)	119.6
C(4)-C(3)-C(2)	120.3(3)
C(4)-C(3)-C(7)	120.7(3)
C(2)-C(3)-C(7)	119.0(3)
C(5)-C(4)-C(3)	118.5(3)
C(5)-C(4)-H(4)	120.7
C(3)-C(4)-H(4)	120.7
C(6)-C(5)-C(4)	121.4(3)
C(6)-C(5)-C(8)	119.1(3)
C(4)-C(5)-C(8)	119.5(3)
C(5)-C(6)-C(1)	120.1(3)
C(5)-C(6)-H(6)	119.9
C(1)-C(6)-H(6)	119.9
F(3)-C(7)-F(2)	106.7(3)
F(3)-C(7)-F(1)	106.3(3)
F(2)-C(7)-F(1)	104.9(3)
F(3)-C(7)-C(3)	113.5(3)
F(2)-C(7)-C(3)	112.4(3)
F(1)-C(7)-C(3)	112.5(3)
F(4)-C(8)-F(6)	106.4(4)
F(4)-C(8)-F(5)	105.4(3)
F(6)-C(8)-F(5)	105.3(3)

F(4)-C(8)-C(5)	113.7(3)
F(6)-C(8)-C(5)	113.5(3)
F(5)-C(8)-C(5)	111.8(4)
C(10)-C(9)-C(14)	119.3(3)
C(10)-C(9)-C(1)	119.2(3)
C(14)-C(9)-C(1)	121.5(3)
C(9)-C(10)-C(11)	122.4(3)
C(9)-C(10)-H(10)	118.8
C(11)-C(10)-H(10)	118.8
C(10)-C(11)-C(12)	117.4(3)
C(10)-C(11)-C(15)	121.3(3)
C(12)-C(11)-C(15)	121.3(3)
C(11)-C(12)-C(13)	122.2(3)
C(11)-C(12)-H(12)	118.9
C(13)-C(12)-H(12)	118.9
C(14)-C(13)-C(12)	118.7(3)
C(14)-C(13)-C(16)	122.9(3)
C(12)-C(13)-C(16)	118.3(3)
C(13)-C(14)-C(9)	120.0(3)
C(13)-C(14)-S(1)	121.7(3)
C(9)-C(14)-S(1)	118.2(3)
C(11)-C(15)-H(15A)	109.5
C(11)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(11)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

O(2)-C(16)-C(13)	111.7(3)
O(2)-C(16)-H(16A)	109.3
C(13)-C(16)-H(16A)	109.3
O(2)-C(16)-H(16B)	109.3
C(13)-C(16)-H(16B)	109.3
H(16A)-C(16)-H(16B)	107.9
O(1)-C(17)-N(1)	123.5(3)
O(1)-C(17)-S(1)	121.2(3)
N(1)-C(17)-S(1)	115.3(3)
N(1)-C(18)-H(18A)	109.5
N(1)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
N(1)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
N(1)-C(19)-H(19A)	109.5
N(1)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
N(1)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-O(2)-H(2D)	102(3)
C(14)-S(1)-C(17)	99.13(17)
C(17)-N(1)-C(19)	123.1(3)
C(17)-N(1)-C(18)	119.4(3)
C(19)-N(1)-C(18)	117.5(3)

Table S3. Crystal data and structure refinement for **3**

Identification code	**3**	
Empirical formula	$C_{41}H_{35}F_{12}IN_4O_2S_2$	
Formula weight	1034.75	
Temperature / K	130(2)	
Wavelength / Å	0.71073	
Crystal system	monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 38.551(2) Å	α = 90°
	b = 5.1209(2) Å	β = 90.316(5)°
	c = 22.0176(10) Å	γ = 90°
Volume / $Å^3$	4346.6(3)	
Z	4	
Density (calculated) / (mg m^{-3})	1.581	
Absorption coefficient / mm^{-1}	0.925	
F(000)	2072	
Crystal size / mm^3	0.540 × 0.070 × 0.060	
Theta range for data collection / degree	3.663-25.349	
Index ranges	$-46 \le h \le 46$, $-6 \le k \le 6$, $-26 \le l \le 26$	
Reflections collected	93543	
Independent reflections	7949 [R(int) = 0.1367]	
Completeness to theta = 25.242° / %	99.8	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	7949 / 0 / 572	
Goodness-of-fit on F^2	1.122	
Final R indices [I > 2sigma(I)]	R_1 = 0.0963, wR_2 = 0.1832	
R indices (all data)	R_1 = 0.1084, wR_2 = 0.1894	
Extinction coefficient	n/a	
Largest diff. peak and hole / $e.Å^{-3}$	1.223 and –2.568	

Table S4. Bond lengths and angles for **3**

Bond length / Å	
S(1)-C(10)	1.777(7)
S(1)-C(20)	1.820(9)
S(2)-C(25)	1.781(8)
S(2)-C(39)	1.814(8)
F(1)-C(18)	1.333(13)
F(2)-C(18)	1.329(10)
F(3)-C(18)	1.344(10)
F(4)-C(19)	1.332(10)
F(5)-C(19)	1.348(9)
F(6)-C(19)	1.325(11)
F(7)-C(37)	1.328(12)
F(8)-C(37)	1.316(11)
F(9)-C(37)	1.309(13)
O(2)-C(39)	1.221(9)
N(1)-C(3)	1.346(10)
N(1)-C(1)	1.366(10)
N(1)-C(23)	1.461(9)
N(2)-C(3)	1.331(9)
N(2)-C(2)	1.371(10)
N(2)-C(4)	1.463(9)
C(1)-C(2)	1.350(11)
C(1)-H(1)	0.9500
C(2)-H(2)	0.9500
C(3)-H(3)	0.9500
C(4)-C(5)	1.524(9)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.384(10)
C(5)-C(10)	1.413(9)
C(6)-C(7)	1.380(10)
C(6)-H(6)	0.9500
C(7)-C(8)	1.404(10)
C(7)-C(11)	1.515(11)
C(8)-C(9)	1.391(10)
C(8)-H(8)	0.9500
C(9)-C(10)	1.417(9)
C(9)-C(12)	1.478(9)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(13)	1.386(10)
C(12)-C(17)	1.393(10)
C(13)-C(14)	1.390(10)
C(13)-H(13)	0.9500
C(14)-C(15)	1.382(11)
C(14)-C(18)	1.491(11)
C(15)-C(16)	1.379(10)
C(15)-H(15)	0.9500
C(16)-C(17)	1.383(10)
C(16)-C(19)	1.501(11)
C(17)-H(17)	0.9500
C(20)-O(1)	1.113(18)
C(20)-N(4P)	1.33(2)
C(20)-N(4)	1.34(2)
C(20)-O(1P)	1.34(2)
C(23)-C(24)	1.516(11)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(29)	1.383(12)
C(24)-C(25)	1.407(10)
C(25)-C(26)	1.390(11)
C(26)-C(27)	1.394(11)
C(26)-C(31)	1.482(10)
C(27)-C(28)	1.390(12)
C(27)-H(27)	0.9500
C(28)-C(29)	1.404(13)
C(28)-C(30)	1.506(12)
C(29)-H(29)	0.9500
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32)	1.382(11)
C(31)-C(36)	1.393(11)
C(32)-C(33)	1.385(11)
C(32)-H(32)	0.9500

C(33)-C(34)	1.394(12)
C(33)-C(37)	1.495(13)
C(34)-C(35)	1.371(13)
C(34)-H(34)	0.9500
C(35)-C(36)	1.384(12)
C(35)-C(38)	1.501(15)
C(36)-H(36)	0.9500
C(38)-F(12P)	1.28(2)
C(38)-F(10)	1.31(4)
C(38)-F(12)	1.35(4)
C(38)-F(11P)	1.35(2)
C(38)-F(10P)	1.351(18)
C(38)-F(11)	1.56(3)
C(39)-N(3)	1.333(10)
N(4)-C(22)	1.47(3)
N(4)-C(21)	1.49(2)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
N(3)-C(40)	1.464(12)
N(3)-C(41)	1.472(12)
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
N(4P)-C(21P)	1.45(3)
N(4P)-C(22P)	1.48(3)
C(21P)-H(21D)	0.9800
C(21P)-H(21E)	0.9800
C(21P)-H(21F)	0.9800
C(22P)-H(22D)	0.9800
C(22P)-H(22E)	0.9800
C(22P)-H(22F)	0.9800

Bond angle / degree	
C(10)-S(1)-C(20)	98.9(4)
C(25)-S(2)-C(39)	98.8(4)
C(3)-N(1)-C(1)	108.2(6)
C(3)-N(1)-C(23)	125.2(7)
C(1)-N(1)-C(23)	126.5(7)
C(3)-N(2)-C(2)	109.5(6)
C(3)-N(2)-C(4)	124.9(6)
C(2)-N(2)-C(4)	125.6(6)
C(2)-C(1)-N(1)	108.2(7)
C(2)-C(1)-H(1)	125.9
N(1)-C(1)-H(1)	125.9
C(1)-C(2)-N(2)	106.4(7)
C(1)-C(2)-H(2)	126.8
N(2)-C(2)-H(2)	126.8
N(2)-C(3)-N(1)	107.8(7)
N(2)-C(3)-H(3)	126.1
N(1)-C(3)-H(3)	126.1
N(2)-C(4)-C(5)	110.8(6)
N(2)-C(4)-H(4A)	109.5
C(5)-C(4)-H(4A)	109.5
N(2)-C(4)-H(4B)	109.5
C(5)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	108.1
C(6)-C(5)-C(10)	120.3(6)
C(6)-C(5)-C(4)	118.5(6)
C(10)-C(5)-C(4)	121.2(6)
C(7)-C(6)-C(5)	121.9(6)
C(7)-C(6)-H(6)	119.1
C(5)-C(6)-H(6)	119.1
C(6)-C(7)-C(8)	117.8(7)
C(6)-C(7)-C(11)	121.4(7)
C(8)-C(7)-C(11)	120.8(7)
C(9)-C(8)-C(7)	122.4(7)
C(9)-C(8)-H(8)	118.8
C(7)-C(8)-H(8)	118.8
C(8)-C(9)-C(10)	118.7(6)
C(8)-C(9)-C(12)	118.8(6)
C(10)-C(9)-C(12)	122.4(6)
C(5)-C(10)-C(9)	118.8(6)
C(5)-C(10)-S(1)	122.5(5)
C(9)-C(10)-S(1)	118.6(5)

C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(13)-C(12)-C(17)	118.1(7)
C(13)-C(12)-C(9)	120.7(7)
C(17)-C(12)-C(9)	121.1(6)
C(12)-C(13)-C(14)	121.2(7)
C(12)-C(13)-H(13)	119.4
C(14)-C(13)-H(13)	119.4
C(15)-C(14)-C(13)	120.2(7)
C(15)-C(14)-C(18)	120.8(7)
C(13)-C(14)-C(18)	119.0(8)
C(16)-C(15)-C(14)	119.0(7)
C(16)-C(15)-H(15)	120.5
C(14)-C(15)-H(15)	120.5
C(15)-C(16)-C(17)	121.0(7)
C(15)-C(16)-C(19)	119.2(7)
C(17)-C(16)-C(19)	119.8(7)
C(16)-C(17)-C(12)	120.6(7)
C(16)-C(17)-H(17)	119.7
C(12)-C(17)-H(17)	119.7
F(2)-C(18)-F(1)	106.4(9)
F(2)-C(18)-F(3)	106.8(8)
F(1)-C(18)-F(3)	105.8(8)
F(2)-C(18)-C(14)	113.2(7)
F(1)-C(18)-C(14)	112.0(8)
F(3)-C(18)-C(14)	112.3(8)
F(6)-C(19)-F(4)	106.9(7)
F(6)-C(19)-F(5)	106.1(7)
F(4)-C(19)-F(5)	106.3(7)
F(6)-C(19)-C(16)	113.1(8)
F(4)-C(19)-C(16)	112.1(7)
F(5)-C(19)-C(16)	111.9(7)
O(1)-C(20)-N(4)	131.6(14)
N(4P)-C(20)-O(1P)	117.1(15)
O(1)-C(20)-S(1)	117.7(11)
N(4P)-C(20)-S(1)	121.6(11)
N(4)-C(20)-S(1)	109.7(10)
O(1P)-C(20)-S(1)	120.6(10)
N(1)-C(23)-C(24)	112.7(6)
N(1)-C(23)-H(23A)	109.1
C(24)-C(23)-H(23A)	109.1
N(1)-C(23)-H(23B)	109.1
C(24)-C(23)-H(23B)	109.1
H(23A)-C(23)-H(23B)	107.8
C(29)-C(24)-C(25)	119.0(7)
C(29)-C(24)-C(23)	118.8(7)
C(25)-C(24)-C(23)	122.0(7)
C(26)-C(25)-C(24)	120.2(7)
C(26)-C(25)-S(2)	120.2(6)
C(24)-C(25)-S(2)	119.6(6)
C(25)-C(26)-C(27)	119.1(7)
C(25)-C(26)-C(31)	122.4(7)
C(27)-C(26)-C(31)	118.4(7)
C(28)-C(27)-C(26)	122.0(8)
C(28)-C(27)-H(27)	119.0
C(26)-C(27)-H(27)	119.0
C(27)-C(28)-C(29)	117.6(8)
C(27)-C(28)-C(30)	120.9(9)
C(29)-C(28)-C(30)	121.5(8)
C(24)-C(29)-C(28)	121.8(8)
C(24)-C(29)-H(29)	119.1
C(28)-C(29)-H(29)	119.1
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(36)	118.7(7)
C(32)-C(31)-C(26)	123.8(7)
C(36)-C(31)-C(26)	117.5(7)
C(31)-C(32)-C(33)	120.7(7)
C(31)-C(32)-H(32)	119.7
C(33)-C(32)-H(32)	119.7
C(32)-C(33)-C(34)	120.4(8)
C(32)-C(33)-C(37)	119.6(8)

C(34)-C(33)-C(37)	120.1(8)
C(35)-C(34)-C(33)	118.8(8)
C(35)-C(34)-H(34)	120.6
C(33)-C(34)-H(34)	120.6
C(34)-C(35)-C(36)	121.1(8)
C(34)-C(35)-C(38)	117.2(9)
C(36)-C(35)-C(38)	121.4(10)
C(35)-C(36)-C(31)	120.3(8)
C(35)-C(36)-H(36)	119.9
C(31)-C(36)-H(36)	119.9
F(9)-C(37)-F(8)	108.7(10)
F(9)-C(37)-F(7)	104.8(9)
F(8)-C(37)-F(7)	104.4(9)
F(9)-C(37)-C(33)	112.4(9)
F(8)-C(37)-C(33)	113.2(8)
F(7)-C(37)-C(33)	112.7(8)
F(10)-C(38)-F(12)	126(2)
F(12P)-C(38)-F(11P)	106.6(12)
F(12P)-C(38)-F(10P)	106.2(16)
F(11P)-C(38)-F(10P)	105.6(14)
F(12P)-C(38)-C(35)	118.1(13)
F(10)-C(38)-C(35)	117.9(16)
F(12)-C(38)-C(35)	114.1(16)
F(11P)-C(38)-C(35)	107.6(15)
F(10P)-C(38)-C(35)	111.9(10)
F(10)-C(38)-F(11)	92(2)
F(12)-C(38)-F(11)	87(2)
C(35)-C(38)-F(11)	105.8(14)
O(2)-C(39)-N(3)	125.5(8)
O(2)-C(39)-S(2)	120.9(6)
N(3)-C(39)-S(2)	113.6(6)
C(20)-N(4)-C(22)	117.7(16)
C(20)-N(4)-C(21)	127.4(15)
C(22)-N(4)-C(21)	114.8(16)
N(4)-C(21)-H(21A)	109.5
N(4)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
N(4)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(4)-C(22)-H(22A)	109.5
N(4)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(4)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(39)-N(3)-C(40)	122.8(8)
C(39)-N(3)-C(41)	119.5(8)
C(40)-N(3)-C(41)	117.5(8)
N(3)-C(40)-H(40A)	109.5
N(3)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
N(3)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
N(3)-C(41)-H(41A)	109.5
N(3)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
N(3)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(20)-N(4P)-C(21P)	121.4(17)
C(20)-N(4P)-C(22P)	123(2)
C(21P)-N(4P)-C(22P)	114.8(19)
N(4P)-C(21P)-H(21D)	109.5
N(4P)-C(21P)-H(21E)	109.5
H(21D)-C(21P)-H(21E)	109.5
N(4P)-C(21P)-H(21F)	109.5
H(21D)-C(21P)-H(21F)	109.5
H(21E)-C(21P)-H(21F)	109.5
N(4P)-C(22P)-H(22D)	109.5
N(4P)-C(22P)-H(22E)	109.5
H(22D)-C(22P)-H(22E)	109.5
N(4P)-C(22P)-H(22F)	109.5
H(22D)-C(22P)-H(22F)	109.5
H(22E)-C(22P)-H(22F)	109.5

Table S5. Crystal data and structure refinement for **4**

Identification code	**4**	
Empirical formula	$C_{44}H_{44}F_{12}N_4O_6S_2$	
Formula weight	1016.95	
Temperature / K	130(2)	
Wavelength / Å	0.71073	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.6705(12) Å	α = 97.743(8)°
	b = 12.6456(13) Å	β = 100.116(10)°
	c = 22.103(2) Å	γ = 100.020(10)°
Volume / $Å^3$	2315.0(5)	
Z	2	
Density (calculated) / (mg m^{-3})	1.459	
Absorption coefficient / mm^{-1}	0.215	
F(000)	1048	
Crystal size / mm^3	0.380 × 0.300 × 0.160	
Theta range for data collection / degree	3.389-25.350	
Index ranges	$-10 \le h \le 10, -15 \le k \le 15, -26 \le l \le 26$	
Reflections collected	22856	
Independent reflections	8467 [R(int) = 0.0332]	
Completeness to theta = 25.242° / %	99.7	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8467 / 102 / 597	
Goodness-of-fit on F^2	1.326	
Final R indices [I > 2sigma(I)]	R_1 = 0.1001, wR_2 = 0.2620	
R indices (all data)	R_1 = 0.1275, wR_2 = 0.2845	
Extinction coefficient	n/a	
Largest diff. peak and hole / e.$Å^{-3}$	1.077 and –0.886	

Table S6. Bond lengths [Å] and angles [°] for **4**

C(1)-O(1)	1.209(7)	C(11)-H(11A)	0.9800
C(1)-N(1)	1.346(7)	C(11)-H(11B)	0.9800
C(1)-S(1)	1.803(5)	C(11)-H(11C)	0.9800
C(1M)-O(1M)	1.365(11)	C(12)-N(3)	1.455(6)
C(1M)-H(1MA)	0.9800	C(12)-C(13)	1.512(7)
C(1M)-H(1MB)	0.9800	C(12)-H(12A)	0.9900
C(1M)-H(1MC)	0.9800	C(12)-H(12B)	0.9900
C(2)-N(1)	1.456(8)	C(13)-C(29)	1.397(7)
C(2)-H(2A)	0.9800	C(13)-C(14)	1.399(6)
C(2)-H(2B)	0.9800	C(14)-C(18)	1.404(6)
C(2)-H(2C)	0.9800	C(14)-S(2)	1.781(4)
C(3)-N(1)	1.445(9)	C(15)-O(5)	1.201(7)
C(3)-H(3A)	0.9800	C(15)-N(4)	1.333(7)
C(3)-H(3B)	0.9800	C(15)-S(2)	1.791(6)
C(3)-H(3C)	0.9800	C(16)-N(4)	1.428(10)
C(4)-C(5)	1.395(6)	C(16)-H(16A)	0.9800
C(4)-C(34)	1.401(6)	C(16)-H(16B)	0.9800
C(4)-S(1)	1.781(4)	C(16)-H(16C)	0.9800
C(5)-C(31)	1.385(7)	C(17)-N(4)	1.470(9)
C(5)-C(6)	1.515(7)	C(17)-H(17A)	0.9800
C(6)-N(2)	1.452(6)	C(17)-H(17B)	0.9800
C(6)-H(6A)	0.9900	C(17)-H(17C)	0.9800
C(6)-H(6B)	0.9900	C(18)-C(27)	1.396(6)
C(7)-O(2)	1.199(7)	C(18)-C(19)	1.494(6)
C(7)-N(3)	1.373(7)	C(19)-C(26)	1.384(7)
C(7)-N(2)	1.378(6)	C(19)-C(20)	1.390(7)
C(8)-N(3)	1.394(8)	C(20)-C(21)	1.386(7)
C(8)-O(3)	1.477(8)	C(20)-H(20)	0.9500
C(8)-C(10)	1.536(8)	C(21)-C(23)	1.380(7)
C(8)-H(8)	1.0000	C(21)-C(22)	1.480(7)
C(9)-O(3)	1.410(10)	C(22)-F(1P)	1.278(9)
C(9)-H(9A)	0.9800	C(22)-F(2)	1.281(9)
C(9)-H(9B)	0.9800	C(22)-F(2P)	1.284(11)
C(9)-H(9C)	0.9800	C(22)-F(3)	1.382(10)
C(10)-O(4)	1.389(8)	C(22)-F(1)	1.399(9)
C(10)-N(2)	1.412(8)	C(22)-F(3P)	1.412(10)
C(10)-H(10)	1.0000	C(23)-C(24)	1.378(7)
C(11)-O(4)	1.422(8)	C(23)-H(23)	0.9500

C(24)-C(26)	1.396(7)	C(41)-F(10P)	1.140(18)
C(24)-C(25)	1.474(7)	C(41)-F(12)	1.290(8)
C(25)-F(6)	1.266(11)	C(41)-F(11)	1.358(9)
C(25)-F(5P)	1.346(12)	C(41)-F(10)	1.390(9)
C(25)-F(6P)	1.388(12)	C(41)-F(12P)	1.410(15)
C(25)-F(4)	1.380(10)	C(41)-F(11P)	1.610(16)
C(25)-F(5)	1.347(12)	C(42)-H(42)	0.9500
C(25)-F(4P)	1.341(11)	C(43)-H(43A)	0.9800
C(26)-H(26)	0.9500	C(43)-H(43B)	0.9800
C(27)-C(28)	1.391(6)	C(43)-H(43C)	0.9800
C(27)-H(27)	0.9500	O(1M)-H(1M)	0.8400
C(28)-C(29)	1.387(7)		
C(28)-C(30)	1.500(7)	O(1)-C(1)-N(1)	124.7(5)
C(29)-H(29)	0.9500	O(1)-C(1)-S(1)	121.4(4)
C(30)-H(30A)	0.9800	N(1)-C(1)-S(1)	113.9(4)
C(30)-H(30B)	0.9800	O(1M)-C(1M)-H(1MA)	109.5
C(30)-H(30C)	0.9800	O(1M)-C(1M)-H(1MB)	109.5
C(31)-C(32)	1.382(8)	H(1MA)-C(1M)-H(1MB)	109.5
C(31)-H(31)	0.9500	O(1M)-C(1M)-H(1MC)	109.5
C(32)-C(33)	1.389(7)	H(1MA)-C(1M)-H(1MC)	109.5
C(32)-C(43)	1.510(7)	H(1MB)-C(1M)-H(1MC)	109.5
C(33)-C(34)	1.393(7)	N(1)-C(2)-H(2A)	109.5
C(33)-H(33)	0.9500	N(1)-C(2)-H(2B)	109.5
C(34)-C(35)	1.495(6)	H(2A)-C(2)-H(2B)	109.5
C(35)-C(42)	1.385(7)	N(1)-C(2)-H(2C)	109.5
C(35)-C(36)	1.391(6)	H(2A)-C(2)-H(2C)	109.5
C(36)-C(37)	1.386(7)	H(2B)-C(2)-H(2C)	109.5
C(36)-H(36)	0.9500	N(1)-C(3)-H(3A)	109.5
C(37)-C(39)	1.379(8)	N(1)-C(3)-H(3B)	109.5
C(37)-C(38)	1.484(8)	H(3A)-C(3)-H(3B)	109.5
C(38)-F(8)	1.248(10)	N(1)-C(3)-H(3C)	109.5
C(38)-F(7)	1.352(11)	H(3A)-C(3)-H(3C)	109.5
C(38)-F(8P)	1.331(9)	H(3B)-C(3)-H(3C)	109.5
C(38)-F(9P)	1.403(10)	C(5)-C(4)-C(34)	120.4(4)
C(38)-F(7P)	1.321(10)	C(5)-C(4)-S(1)	119.4(4)
C(38)-F(9)	1.392(12)	C(34)-C(4)-S(1)	119.9(3)
C(39)-C(40)	1.381(8)	C(31)-C(5)-C(4)	119.0(4)
C(39)-H(39)	0.9500	C(31)-C(5)-C(6)	121.4(4)
C(40)-C(42)	1.391(7)	C(4)-C(5)-C(6)	119.5(4)
C(40)-C(41)	1.483(8)	N(2)-C(6)-C(5)	114.1(4)

N(2)-C(6)-H(6A)	108.7
C(5)-C(6)-H(6A)	108.7
N(2)-C(6)-H(6B)	108.7
C(5)-C(6)-H(6B)	108.7
H(6A)-C(6)-H(6B)	107.6
O(2)-C(7)-N(3)	127.3(5)
O(2)-C(7)-N(2)	126.5(5)
N(3)-C(7)-N(2)	106.1(5)
N(3)-C(8)-O(3)	105.1(5)
N(3)-C(8)-C(10)	103.8(5)
O(3)-C(8)-C(10)	110.9(5)
N(3)-C(8)-H(8)	112.2
O(3)-C(8)-H(8)	112.2
C(10)-C(8)-H(8)	112.2
O(3)-C(9)-H(9A)	109.5
O(3)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
O(3)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
O(4)-C(10)-N(2)	117.4(5)
O(4)-C(10)-C(8)	107.3(5)
N(2)-C(10)-C(8)	101.7(5)
O(4)-C(10)-H(10)	110.0
N(2)-C(10)-H(10)	110.0
C(8)-C(10)-H(10)	110.0
O(4)-C(11)-H(11A)	109.5
O(4)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(4)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(3)-C(12)-C(13)	113.5(4)
N(3)-C(12)-H(12A)	108.9
C(13)-C(12)-H(12A)	108.9
N(3)-C(12)-H(12B)	108.9
C(13)-C(12)-H(12B)	108.9
H(12A)-C(12)-H(12B)	107.7
C(29)-C(13)-C(14)	118.8(4)
C(29)-C(13)-C(12)	120.2(4)
C(14)-C(13)-C(12)	120.9(4)
C(13)-C(14)-C(18)	120.2(4)
C(13)-C(14)-S(2)	118.8(4)
C(18)-C(14)-S(2)	120.3(3)
O(5)-C(15)-N(4)	124.9(6)
O(5)-C(15)-S(2)	121.2(5)
N(4)-C(15)-S(2)	113.9(5)
N(4)-C(16)-H(16A)	109.5
N(4)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
N(4)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
N(4)-C(17)-H(17A)	109.5
N(4)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
N(4)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(27)-C(18)-C(14)	119.0(4)
C(27)-C(18)-C(19)	117.9(4)
C(14)-C(18)-C(19)	123.0(4)
C(26)-C(19)-C(20)	118.5(4)
C(26)-C(19)-C(18)	119.7(4)
C(20)-C(19)-C(18)	121.8(4)
C(21)-C(20)-C(19)	120.4(4)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(23)-C(21)-C(20)	120.6(5)
C(23)-C(21)-C(22)	119.4(4)
C(20)-C(21)-C(22)	119.9(5)
F(1P)-C(22)-F(2P)	112.1(7)
F(2)-C(22)-F(3)	107.3(6)
F(2)-C(22)-F(1)	102.9(6)
F(3)-C(22)-F(1)	102.7(6)
F(1P)-C(22)-F(3P)	104.6(7)
F(2P)-C(22)-F(3P)	105.5(6)
F(1P)-C(22)-C(21)	112.2(5)
F(2)-C(22)-C(21)	116.5(6)
F(2P)-C(22)-C(21)	113.5(6)

F(3)-C(22)-C(21)	111.6(5)
F(1)-C(22)-C(21)	114.5(5)
F(3P)-C(22)-C(21)	108.3(5)
C(24)-C(23)-C(21)	119.7(4)
C(24)-C(23)-H(23)	120.1
C(21)-C(23)-H(23)	120.1
C(23)-C(24)-C(26)	119.5(5)
C(23)-C(24)-C(25)	120.3(5)
C(26)-C(24)-C(25)	120.2(5)
F(5P)-C(25)-F(6P)	107.1(6)
F(6)-C(25)-F(4)	107.5(6)
F(6)-C(25)-F(5)	107.6(7)
F(4)-C(25)-F(5)	106.9(6)
F(5P)-C(25)-F(4P)	105.7(6)
F(6P)-C(25)-F(4P)	102.9(7)
F(6)-C(25)-C(24)	113.0(6)
F(5P)-C(25)-C(24)	110.9(6)
F(6P)-C(25)-C(24)	113.6(5)
F(4)-C(25)-C(24)	108.5(6)
F(5)-C(25)-C(24)	113.0(6)
F(4P)-C(25)-C(24)	115.8(6)
C(19)-C(26)-C(24)	121.2(5)
C(19)-C(26)-H(26)	119.4
C(24)-C(26)-H(26)	119.4
C(28)-C(27)-C(18)	121.8(4)
C(28)-C(27)-H(27)	119.1
C(18)-C(27)-H(27)	119.1
C(29)-C(28)-C(27)	118.1(4)
C(29)-C(28)-C(30)	121.5(4)
C(27)-C(28)-C(30)	120.4(4)
C(28)-C(29)-C(13)	122.1(4)
C(28)-C(29)-H(29)	119.0
C(13)-C(29)-H(29)	119.0
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(5)	121.9(4)
C(32)-C(31)-H(31)	119.1
C(5)-C(31)-H(31)	119.1
C(31)-C(32)-C(33)	118.5(4)
C(31)-C(32)-C(43)	120.9(5)
C(33)-C(32)-C(43)	120.5(5)
C(32)-C(33)-C(34)	121.5(5)
C(32)-C(33)-H(33)	119.3
C(34)-C(33)-H(33)	119.3
C(33)-C(34)-C(4)	118.6(4)
C(33)-C(34)-C(35)	117.7(4)
C(4)-C(34)-C(35)	123.4(4)
C(42)-C(35)-C(36)	118.3(4)
C(42)-C(35)-C(34)	120.9(4)
C(36)-C(35)-C(34)	120.5(4)
C(37)-C(36)-C(35)	120.6(5)
C(37)-C(36)-H(36)	119.7
C(35)-C(36)-H(36)	119.7
C(39)-C(37)-C(36)	120.8(5)
C(39)-C(37)-C(38)	119.9(5)
C(36)-C(37)-C(38)	119.2(5)
F(8)-C(38)-F(7)	111.4(7)
F(8P)-C(38)-F(9P)	110.0(6)
F(8P)-C(38)-F(7P)	104.5(7)
F(9P)-C(38)-F(7P)	104.5(6)
F(8)-C(38)-F(9)	100.1(7)
F(7)-C(38)-F(9)	107.4(7)
F(8)-C(38)-C(37)	117.7(6)
F(7)-C(38)-C(37)	109.0(6)
F(8P)-C(38)-C(37)	114.8(5)
F(9P)-C(38)-C(37)	111.0(6)
F(7P)-C(38)-C(37)	111.4(6)
F(9)-C(38)-C(37)	110.6(6)
C(37)-C(39)-C(40)	119.0(5)
C(37)-C(39)-H(39)	120.5
C(40)-C(39)-H(39)	120.5
C(39)-C(40)-C(42)	120.4(5)
C(39)-C(40)-C(41)	119.8(5)
C(42)-C(40)-C(41)	119.8(5)
F(12)-C(41)-F(11)	108.1(6)
F(12)-C(41)-F(10)	104.5(5)

F(11)-C(41)-F(10)	103.2(6)
F(10P)-C(41)-F(12P)	133.0(12)
F(10P)-C(41)-C(40)	117.5(10)
F(12)-C(41)-C(40)	114.4(6)
F(11)-C(41)-C(40)	114.1(5)
F(10)-C(41)-C(40)	111.5(5)
F(12P)-C(41)-C(40)	109.4(7)
F(10P)-C(41)-F(11P)	92.2(11)
F(12P)-C(41)-F(11P)	75.7(9)
C(40)-C(41)-F(11P)	101.1(7)
C(40)-C(42)-C(35)	120.9(5)
C(40)-C(42)-H(42)	119.6
C(35)-C(42)-H(42)	119.6
C(32)-C(43)-H(43A)	109.5
C(32)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(32)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(1)-N(1)-C(3)	124.3(5)
C(1)-N(1)-C(2)	117.2(6)
C(3)-N(1)-C(2)	118.0(5)
C(7)-N(2)-C(10)	112.7(4)
C(7)-N(2)-C(6)	121.6(4)
C(10)-N(2)-C(6)	124.8(4)
C(7)-N(3)-C(8)	110.7(4)
C(7)-N(3)-C(12)	122.0(5)
C(8)-N(3)-C(12)	121.6(5)
C(15)-N(4)-C(16)	124.3(6)
C(15)-N(4)-C(17)	118.2(6)
C(16)-N(4)-C(17)	117.5(6)
C(1M)-O(1M)-H(1M)	109.5
C(9)-O(3)-C(8)	112.8(7)
C(10)-O(4)-C(11)	115.6(5)
C(4)-S(1)-C(1)	100.4(2)
C(14)-S(2)-C(15)	101.5(2)

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

```
Bond precision:  C-C = 0.0050 A          Wavelength=0.71073

Cell:           a=5.134(2)        b=10.620(4)      c=17.878(4)
                alpha=99.45(2)    beta=96.43(3)    gamma=93.37(3)
Temperature:    130 K

                Calculated                Reported
Volume          952.5(6)                  952.6(6)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C19 H17 F6 N O2 S         C19 H17 F6 N1 O2
S1 Sum formula  C19 H17 F6 N O2 S         C19 H17 F6 N O2
S Mr            437.40                    437.40
Dx,g cm-3       1.525                     1.525
Z               2                         2
Mu (mm-1)       0.242                     0.242
F000            448.0                     448.0
F000'           448.58
h,k,lmax        6,12,21                   6,12,21
Nref            3371                      3362
Tmin,Tmax       0.976,0.981               0.950,0.982
Tmin'           0.927

Correction method= # Reported T Limits: Tmin=0.950
Tmax=0.982 AbsCorr = ANALYTICAL

Data completeness= 0.997          Theta(max)= 25.030

R(reflections)= 0.0583( 2244)     wR2(reflections)= 0.1594( 3362)

S = 1.059                 Npar= 268
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT340 ALERT 3 C Low Bond Precision on C-C Bonds ..... 0.005 Ang.

Alert level G

PLAT002 ALERT 2 G Number of Distance or Angle Restraints on AtSite 2
PLAT005 ALERT 5 G Note No Embedded Refinement Details Found in the
PLAT242 ALERT 2 G CIF Please Do ! Low 'MainMol' Ueq as
PLAT242 ALERT 2 G Compared to Neighbors of C7 Check
PLAT860 ALERT 3 G Low 'MainMol' Ueq as Compared to Neighbors of C8
Check Number of Least-Squares Restraints 1
Note

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0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL012_ALERT_1_A _publ_section_abstract is
missing.
Abstract of paper in English.

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Publication of your CIF

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Validation response form

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```
# start Validation Reply Form
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

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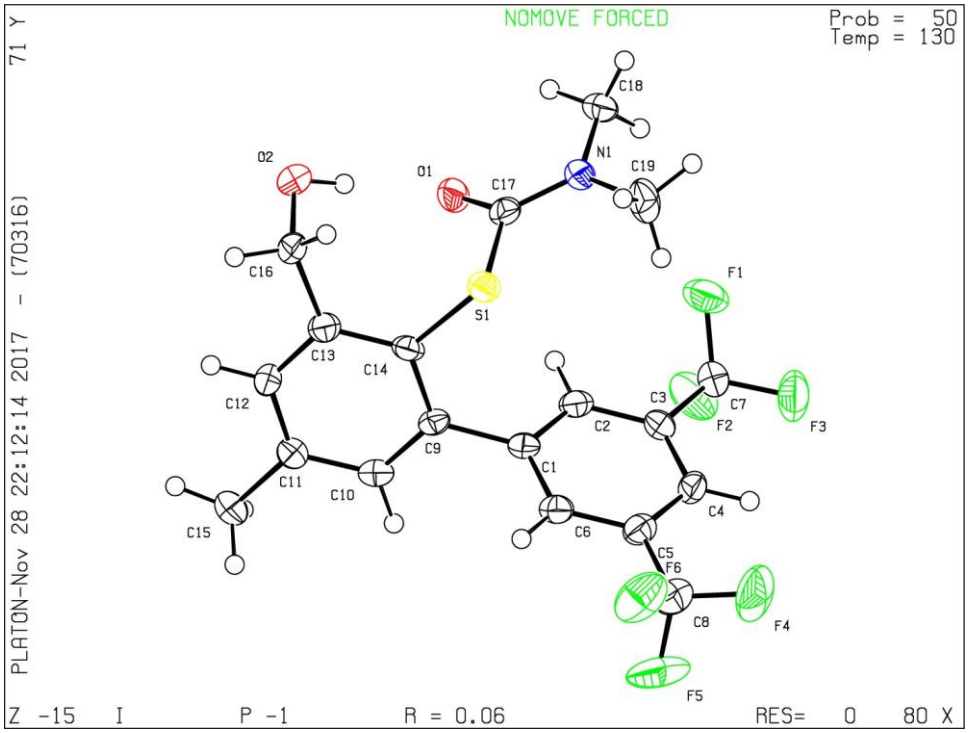
PLATON version of 09/11/2017; check.def file version of 08/11/2017

Datablock I - ellipsoid plot



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0111 A Wavelength=0.71073

Cell: a=38.551(2) b=5.1209(2) c=22.0176(10)
alpha=90 beta=90.316(5) gamma=90
Temperature: 130 K

	Calculated	Reported
Volume	4346.6(3)	4346.6(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C41 H35 F12 N4 O2 S2, I	C41 H35 F12 N4 O2 S2, I
Sum formula	C41 H35 F12 I N4 O2 S2	C41 H35 F12 I N4 O2 S2
Mr	1034.75	1034.75
Dx,g cm-3	1.581	1.581
Z	4	4
Mu (mm-1)	0.925	0.925
F000	2072.0	2072.0
F000'	2072.40	
h,k,lmax	46,6,26	46,6,26
Nref	7966	7949
Tmin,Tmax	0.925,0.946	0.533,0.876
Tmin'	0.607	

Correction method= # Reported T Limits: Tmin=0.533
Tmax=0.876 AbsCorr = ANALYTICAL

Data completeness= 0.998 Theta(max)= 25.349

R(reflections)= 0.0963(6714) wR2(reflections)= 0.1894(7949)

S = 1.122 Npar= 572

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.137

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.137 Report
PLAT213_ALERT_2_C	Atom F2 has ADP max/min Ratio	3.1 prolat
PLAT213_ALERT_2_C	Atom F3 has ADP max/min Ratio	3.1 prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	5.1 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference F10 -- C38	0.19 Ang.
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)	O1P Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01114 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4B ..I1	3.09 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H21B ..F2	2.65 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H22B ..I1	3.09 Ang.

Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Foundin the CIFPlease Do !
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large 68.88
PLAT230_ALERT_2_G	Why ? Hirshfeld Test Diff for F10P --C38 ..
PLAT230_ALERT_2_G	7.8 s.u. Hirshfeld Test Diff forF12P --C38
PLAT242_ALERT_2_G	.. 6.7 s.u. Hirshfeld Test
PLAT242_ALERT_2_G	Diff for F12 --C38 .. 6.6
PLAT242_ALERT_2_G	s.u. Low 'MainMol' Ueq as Compared to Neighbors of
PLAT301_ALERT_3_G	C18 Check Low 'MainMol' Ueq as Compared to
PLAT434_ALERT_2_G	Neighbors of C19 Check Low
PLAT790_ALERT_4_G	'MainMol' Ueq as Compared to Neighbors of C37
	Check Main Residue Disorder .....(Resd 1)
	11% Note Short Inter HL..HL Contact
	F8 ..F12 2.75 Ang.
	Centre of Gravity not Within Unit Cell: Resd. # 2
	Note
	I

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11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

---

checkCIF publication errors

Alert level A

PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

---

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---

Publication of your CIF

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Validation response form

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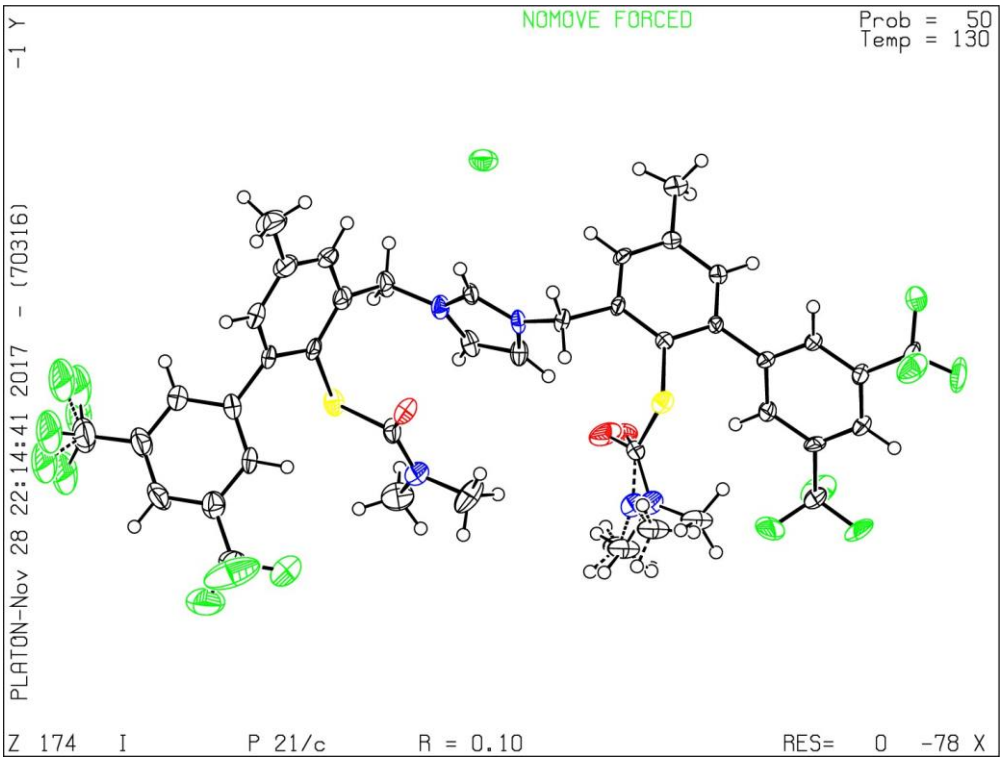
```
# start Validation Reply Form
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 09/11/2017; check.def file version of 08/11/2017

Datablock I - ellipsoid plot



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

```
Bond precision:  C-C = 0.0070 A          Wavelength=0.71073

Cell:          a=8.6705(12)      b=12.6456(13)      c=22.103(2)
               alpha=97.743(8)   beta=100.116(10)   gamma=100.02(1)
Temperature:   130 K
```

	Calculated	Reported
Volume	2315.0(5)	2315.0(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C43 H40 F12 N4 O5 S2, C H4 O	?
Sum formula	C44 H44 F12 N4 O6 S2	C44 H44 F12 N4 O6 S2
Mr	1016.95	1016.95
Dx,g cm-3	1.459	1.459
Z	2	2
Mu (mm-1)	0.215	0.215
F000	1048.0	1048.0
F000'	1049.23	
h,k,lmax	10,15,26	10,15,26
Nref	8492	8467
Tmin,Tmax	0.926,0.966	0.937,0.968
Tmin'	0.922	

```
Correction method= # Reported T Limits: Tmin=0.937 Tmax=0.968
AbsCorr = ANALYTICAL

Data completeness= 0.997          Theta(max)= 25.350

R(reflections)= 0.1001( 6318)     wR2(reflections)= 0.2845( 8467)

S = 1.326                 Npar= 597
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT048_ALERT_1_C MoietyFormula Not Given (or Incomplete) ..... Please
PLAT084_ALERT_3_C Check High wR2 Value (i.e. > 0.25) .....
PLAT220_ALERT_2_C 0.28
PLAT222_ALERT_3_C Report
PLAT242_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.5 Ratio Non-
PLAT340_ALERT_3_C Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.0 Ratio
Low 'MainMol' Ueq as Compared to Neighbors of N4 Check
Low Bond Precision on C-C Bonds ..... 0.00697 Ang.

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 24
PLAT005_ALERT_5_G Report No Embedded Refinement Details Found in the CIF Please
PLAT007_ALERT_5_G Do !
PLAT072_ALERT_2_G Number of Unrefined Donor-H Atoms ..... 1 Report
PLAT230_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for F2 --C22 .. 15.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for F3 --C22 .. 10.7
PLAT230_ALERT_2_G s.u. Hirshfeld Test Diff for F5 --C25 ..
PLAT230_ALERT_2_G 12.0 s.u. Hirshfeld Test Diff for
PLAT230_ALERT_2_G F12 --C41 .. 9.8
PLAT230_ALERT_2_G s.u. Hirshfeld Test Diff for F2P --C22 ..
PLAT230_ALERT_2_G 10.7 s.u. Hirshfeld Test Diff for
PLAT242_ALERT_2_G F3P --C22 .. 11.3
PLAT242_ALERT_2_G s.u. Hirshfeld Test Diff for F4P --C25 ..
PLAT301_ALERT_3_G 5.7 s.u. Hirshfeld Test Diff for
PLAT432_ALERT_2_G F5P --C25 .. 14.7
PLAT720_ALERT_4_G s.u. Hirshfeld Test Diff for F8 --C38 ..
PLAT790_ALERT_4_G 6.3 s.u. Hirshfeld Test Diff for
F12P --C41 .. 9.8 s.u. Low 'MainMol' Ueq as
Compared to Neighbors of C22 Check Low 'MainMol' Ueq as
Compared to Neighbors of C25 Check Main Residue Disorder
.....(Resd 1) 18% Note Short Inter X...Y
Contact O5 ..C1M 3.02 Ang. Number of
Unusual/Non-Standard Labels ..... 3 Note Centre of
Gravity not Within Unit Cell: Resd. # 2 Note
C H4 O
PLAT793_ALERT_4_G Model has Chirality at C8 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C10 (Centro SPGR) S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 102 Note

---

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---

checkCIF publication errors

Alert level A

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Abstract of paper in English.

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```
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;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

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Datablock I - ellipsoid plot