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**

| Parameter                                      | Value                        |
|------------------------------------------------|------------------------------|
| Identification code                            | 1                            |
| Empirical formula                              | C_{19}H_{17}F_{6}NO_{2}S     |
| 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               |
|                                                | b = 10.620(4) Å              |
|                                                | c = 17.878(4) Å              |
|                                                | α = 99.45(2)°                |
|                                                | β = 96.43(3)°                |
|                                                | γ = 93.37(3)°                |
| Volume / Å³                                     | 952.6(6)                     |
| Z                                              | 2                            |
| Density (calculated) / (mg m⁻³)                 | 1.525                        |
| Absorption coefficient / mm⁻¹                   | 0.242                        |
| F(000)                                         | 448                          |
| Crystal size / mm³                              | 0.54 × 0.07 × 0.06           |
| Theta range for data collection / degree        | 3.49-25.03                   |
| Index ranges                                   | −6 ≤ h ≤ 6, −12 ≤ k ≤ 11, −21 ≤ l ≤ 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 F² |
| Data / restraints / parameters                  | 3362 / 1 / 268               |
| Goodness-of-fit on F²                           | 1.059                        |
| Final R indices [I > 2σ(I)]                    | R₁ = 0.0583, wR₂ = 0.1281    |
| R indices (all data)                            | R₁ = 0.0972, wR₂ = 0.1594    |
| Largest diff. peak and hole / e.Å⁻³            | 0.340 and −0.344             |
|      | Bond length / Å | C(17)-S(1) | 1.811(4) |
|------|----------------|------------|----------|
| C(1)-C(2) | 1.388(5) | C(18)-N(1) | 1.471(5) |
| C(1)-C(6) | 1.391(5) | C(18)-H(18A) | 0.9800 |
| C(1)-C(9) | 1.502(5) | C(18)-H(18B) | 0.9800 |
| C(2)-C(3) | 1.393(5) | C(18)-H(18C) | 0.9800 |
| C(2)-H(2) | 0.9500 | C(19)-N(1) | 1.459(5) |
| C(3)-C(4) | 1.390(5) | C(19)-H(19A) | 0.9800 |
| C(3)-C(7) | 1.494(5) | C(19)-H(19B) | 0.9800 |
| C(4)-C(5) | 1.387(5) | C(19)-H(19C) | 0.9800 |
| C(4)-H(4) | 0.9500 | O(2)-H(2D) | 0.876(19) |
| C(5)-C(6) | 1.385(5) | C(2)-C(1)-C(6) | 118.9(3) |
| C(5)-C(8) | 1.495(5) | C(2)-C(1)-C(9) | 119.7(3) |
| C(6)-H(6) | 0.9500 | C(6)-C(1)-C(9) | 121.5(3) |
| C(7)-F(3) | 1.328(4) | C(1)-C(2)-C(3) | 120.8(3) |
| C(7)-F(2) | 1.336(5) | C(1)-C(2)-H(2) | 119.6 |
| C(7)-F(1) | 1.342(4) | C(3)-C(2)-H(2) | 119.6 |
| C(8)-F(4) | 1.325(5) | C(4)-C(3)-C(2) | 120.3(3) |
| C(8)-F(6) | 1.334(5) | C(4)-C(3)-C(7) | 120.7(3) |
| C(9)-C(10) | 1.382(5) | C(2)-C(3)-C(7) | 119.0(3) |
| C(9)-C(14) | 1.408(5) | C(5)-C(4)-C(3) | 118.5(3) |
| C(10)-C(11) | 1.386(5) | C(5)-C(4)-H(4) | 120.7 |
| C(10)-H(10) | 0.9500 | C(3)-C(4)-H(4) | 120.7 |
| C(11)-C(12) | 1.397(5) | C(6)-C(5)-C(4) | 121.4(3) |
| C(11)-C(15) | 1.496(5) | C(6)-C(5)-C(8) | 119.1(3) |
| C(12)-C(13) | 1.400(5) | C(4)-C(5)-C(8) | 119.5(3) |
| C(12)-H(12) | 0.9500 | C(5)-C(6)-C(1) | 120.1(3) |
| C(13)-C(14) | 1.393(5) | C(5)-C(6)-H(6) | 119.9 |
| C(13)-C(16) | 1.514(5) | C(1)-C(6)-H(6) | 119.9 |
| C(14)-S(1) | 1.787(4) | F(3)-C(7)-F(2) | 106.7(3) |
| C(15)-H(15A) | 0.9800 | F(3)-C(7)-F(1) | 106.3(3) |
| C(15)-H(15B) | 0.9800 | F(2)-C(7)-F(1) | 104.9(3) |
| C(15)-H(15C) | 0.9800 | F(3)-C(7)-C(3) | 113.5(3) |
| C(16)-O(2) | 1.432(4) | F(2)-C(7)-C(3) | 112.4(3) |
| C(16)-H(16A) | 0.9900 | F(1)-C(7)-C(3) | 112.5(3) |
| C(16)-H(16B) | 0.9900 | F(4)-C(8)-F(6) | 106.4(4) |
| C(17)-O(1) | 1.228(4) | F(4)-C(8)-F(5) | 105.4(3) |
| C(17)-N(1) | 1.346(4) | F(6)-C(8)-F(5) | 105.3(3) |
| Bond                  | Angle (°)   |
|----------------------|------------|
| 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(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(15)-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)   |
| N(1)-C(17)-S(1)      | 121.2(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      |
| O(1)-C(17)-N(1)      | 115.3(3)   |
| O(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      |
| 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

|                                | 3                                           |
|--------------------------------|---------------------------------------------|
| Identification code            | C41H35F12IN3O2S2                            |
| Empirical formula              | C41H35F12IN3O2S2                            |
| 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 / Å³                    | 4346.6(3)                                   |
| Z                              | 4                                           |
| Density (calculated) / (mg m³) | 1.581                                       |
| Absorption coefficient / mm⁻¹  | 0.925                                       |
| F(000)                         | 2072                                        |
| Crystal size / mm³             | 0.540 × 0.070 × 0.060                       |
| Theta range for data collection / degree | 3.663-25.349                             |
| Index ranges                   | -46 ≤ h ≤ 46, -6 ≤ k ≤ 6, -26 ≤ l ≤ 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 F²            |
| Data / restraints / parameters | 7949 / 0 / 572                              |
| Goodness-of-fit on F²          | 1.122                                       |
| Final R indices [I > 2σ(I)]    | R₁ = 0.0963, wR₂ = 0.1832                   |
| R indices (all data)           | R₁ = 0.1084, wR₂ = 0.1894                   |
| Extinction coefficient         | n/a                                         |
| Largest diff. peak and hole / e.Å⁻³ | 1.223 and -2.568                         |
| Bond length / Å | C(11)-H(11A) | 0.9800 |
|----------------|---------------|---------|
| 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(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(10)    | 1.478(9)      |         |
| 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        |         |
| Bond          | Distance  | Bond          | Distance  |
|---------------|-----------|---------------|-----------|
| C(33)-C(34)   | 1.394(12) | C(25)-S(2)-C(39) | 98.8(4)   |
| C(33)-C(37)   | 1.495(13) | C(3)-N(1)-C(1)   | 108.2(6)  |
| C(34)-C(35)   | 1.371(13) | C(3)-N(1)-C(23)  | 125.2(7)  |
| C(34)-H(34)   | 0.9500    | C(1)-N(1)-C(23)  | 126.5(7)  |
| C(35)-C(36)   | 1.384(12) | C(3)-N(2)-C(2)   | 109.5(6)  |
| C(35)-C(38)   | 1.501(15) | C(3)-N(2)-C(4)   | 124.9(6)  |
| C(36)-H(36)   | 0.9500    | C(2)-N(2)-C(4)   | 125.6(6)  |
| C(38)-F(12P)  | 1.28(2)   | C(2)-C(1)-N(1)   | 108.2(7)  |
| C(38)-F(10)   | 1.31(4)   | C(2)-C(1)-H(1)   | 125.9     |
| C(38)-F(12)   | 1.35(4)   | N(1)-C(1)-H(1)   | 125.9     |
| C(38)-F(11P)  | 1.35(2)   | C(1)-C(2)-N(2)   | 106.4(7)  |
| C(38)-F(10P)  | 1.351(18) | C(1)-C(2)-H(2)   | 126.8     |
| C(38)-F(11)   | 1.56(3)   | N(2)-C(2)-H(2)   | 126.8     |
| C(39)-N(3)    | 1.333(10) | N(2)-C(3)-N(1)   | 107.8(7)  |
| N(4)-C(22)    | 1.47(3)   | N(2)-C(3)-H(3)   | 126.1     |
| N(4)-C(21)    | 1.49(2)   | N(1)-C(3)-H(3)   | 126.1     |
| C(21)-H(21A)  | 0.9800    | N(2)-C(4)-C(5)   | 110.8(6)  |
| C(21)-H(21B)  | 0.9800    | N(2)-C(4)-H(4A)  | 109.5     |
| C(21)-H(21C)  | 0.9800    | C(5)-C(4)-H(4A)  | 109.5     |
| C(22)-H(22A)  | 0.9800    | N(2)-C(4)-H(4B)  | 109.5     |
| C(22)-H(22B)  | 0.9800    | C(5)-C(4)-H(4B)  | 109.5     |
| C(22)-H(22C)  | 0.9800    | H(4A)-C(4)-H(4B) | 108.1     |
| N(3)-C(40)    | 1.464(12) | C(6)-C(5)-C(10)  | 120.3(6)  |
| N(3)-C(41)    | 1.472(12) | C(6)-C(5)-C(4)   | 118.5(6)  |
| C(40)-H(40A)  | 0.9800    | C(10)-C(5)-C(4)  | 121.2(6)  |
| C(40)-H(40B)  | 0.9800    | C(7)-C(6)-C(5)   | 121.9(6)  |
| C(40)-H(40C)  | 0.9800    | C(7)-C(6)-H(6)   | 119.1     |
| C(41)-H(41A)  | 0.9800    | C(5)-C(6)-H(6)   | 119.1     |
| C(41)-H(41B)  | 0.9800    | C(6)-C(7)-C(8)   | 117.8(7)  |
| C(41)-H(41C)  | 0.9800    | C(6)-C(7)-C(11)  | 121.4(7)  |
| N(4P)-C(21P)  | 1.45(3)   | C(8)-C(7)-C(11)  | 120.8(7)  |
| N(4P)-C(22P)  | 1.48(3)   | C(9)-C(8)-C(7)   | 122.4(7)  |
| C(21P)-H(21D) | 0.9800    | C(9)-C(8)-H(8)   | 118.8     |
| C(21P)-H(21E) | 0.9800    | C(7)-C(8)-H(8)   | 118.8     |
| C(21P)-H(21F) | 0.9800    | C(8)-C(9)-C(10)  | 118.7(6)  |
| C(22P)-H(22D) | 0.9800    | C(8)-C(9)-C(12)  | 118.8(6)  |
| C(22P)-H(22E) | 0.9800    | C(10)-C(9)-C(12) | 122.4(6)  |
| C(22P)-H(22F) | 0.9800    | C(5)-C(10)-C(9)  | 118.8(6)  |

| Bond angle / degree |
|---------------------|
| Bond              | Angle     |
| C(10)-S(1)-C(20)   | 98.9(4)   |
| C(9)-C(10)-S(1)    | 122.5(5)  |
| C(9)-C(10)-S(1)    | 118.6(5)  |
| Bond                        | Angle   | Bond                        | Angle   |
|-----------------------------|---------|-----------------------------|---------|
| C(7)-C(11)-H(11A)          | 109.5   | N(4)-C(20)-S(1)             | 109.7(10) |
| C(7)-C(11)-H(11B)          | 109.5   | O(1P)-C(20)-S(1)            | 120.6(10) |
| H(11A)-C(11)-H(11B)        | 109.5   | N(1)-C(23)-S(1)             | 112.7(6)  |
| C(7)-C(11)-H(11C)          | 109.5   | N(1)-C(23)-H(23A)           | 109.1    |
| H(11A)-C(11)-H(11C)        | 109.5   | C(24)-C(23)-H(23A)          | 109.1    |
| H(11B)-C(11)-H(11C)        | 109.5   | N(1)-C(23)-H(23B)           | 109.1    |
| C(13)-C(12)-C(17)          | 118.1(7) | C(24)-C(23)-H(23B)          | 109.1    |
| C(13)-C(12)-C(9)           | 120.7(7) | C(24A)-C(23)-H(23B)         | 107.8    |
| C(17)-C(12)-C(9)           | 121.1(6) | C(29)-C(24)-C(25)           | 119.0(7)  |
| C(12)-C(13)-C(14)          | 121.2(7) | C(29)-C(24)-C(23)           | 118.8(7)  |
| C(12)-C(13)-H(13)          | 119.4   | C(25)-C(24)-C(23)           | 122.0(7)  |
| C(14)-C(13)-H(13)          | 119.4   | C(26)-C(25)-C(24)           | 120.2(7)  |
| C(15)-C(14)-C(13)          | 120.2(7) | C(26)-C(25)-S(2)            | 120.2(6)  |
| C(15)-C(14)-C(18)          | 120.8(7) | C(24)-C(25)-S(2)            | 119.6(6)  |
| C(13)-C(14)-C(18)          | 119.0(8) | C(25)-C(26)-C(27)           | 119.1(7)  |
| C(16)-C(15)-C(14)          | 119.0(7) | C(25)-C(26)-C(31)           | 122.4(7)  |
| C(16)-C(15)-H(15)          | 120.5   | C(27)-C(26)-C(31)           | 118.4(7)  |
| C(14)-C(15)-H(15)          | 120.5   | C(27)-C(26)-C(26)           | 122.0(8)  |
| C(15)-C(16)-C(17)          | 121.0(7) | C(28)-C(27)-H(27)           | 119.0    |
| C(15)-C(16)-C(19)          | 119.2(7) | C(26)-C(27)-H(27)           | 119.0    |
| C(17)-C(16)-C(19)          | 119.8(7) | C(27)-C(28)-C(29)           | 117.6(8)  |
| C(16)-C(17)-C(12)          | 120.6(7) | C(27)-C(28)-C(30)           | 120.9(9)  |
| C(16)-C(17)-H(17)          | 119.7   | C(29)-C(28)-C(30)           | 121.5(8)  |
| C(12)-C(17)-H(17)          | 119.7   | C(24)-C(29)-C(28)           | 121.8(8)  |
| F(2)-C(18)-F(1)            | 106.4(9) | C(24)-C(29)-H(29)           | 119.1    |
| F(2)-C(18)-F(3)            | 106.8(8) | C(28)-C(29)-H(29)           | 119.1    |
| F(1)-C(18)-F(3)            | 105.8(8) | C(28)-C(30)-H(30A)          | 109.5    |
| F(2)-C(18)-C(14)           | 113.2(7) | C(28)-C(30)-H(30B)          | 109.5    |
| F(1)-C(18)-C(14)           | 112.0(8) | H(30A)-C(30)-H(30B)         | 109.5    |
| F(3)-C(18)-C(14)           | 112.3(8) | C(28)-C(30)-H(30C)          | 109.5    |
| F(6)-C(19)-F(4)            | 106.9(7) | H(30A)-C(30)-H(30C)         | 109.5    |
| F(6)-C(19)-F(5)            | 106.1(7) | H(30B)-C(30)-H(30C)         | 109.5    |
| F(4)-C(19)-F(5)            | 106.3(7) | C(32)-C(31)-C(36)           | 118.7(7)  |
| F(6)-C(19)-C(16)           | 113.1(8) | C(32)-C(31)-C(26)           | 123.8(7)  |
| F(4)-C(19)-C(16)           | 112.1(7) | C(36)-C(31)-C(26)           | 117.5(7)  |
| F(5)-C(19)-C(16)           | 111.9(7) | C(31)-C(32)-C(33)           | 120.7(7)  |
| O(1)-C(20)-N(4)            | 131.6(14)| C(31)-C(32)-H(32)           | 119.7    |
| N(4P)-C(20)-O(1P)          | 117.1(15)| C(33)-C(32)-H(32)           | 119.7    |
| O(1)-C(20)-S(1)            | 117.7(11)| C(32)-C(33)-C(34)           | 120.4(8)  |
| N(4P)-C(20)-S(1)           | 121.6(11)| C(32)-C(33)-C(37)           | 119.6(8)  |
| Bond | Angle |
|------|-------|
| 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) | 117.2(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(11P)-C(38)-C(35) | 114.1(16) |
| F(10P)-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 |

| Bond | Angle |
|------|-------|
| 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(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) |
| H(21D)-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 |
| Identification code | 4 |
|---------------------|---|
| Empirical formula   | C_{44}H_{44}F_{12}N_{4}O_{6}S_{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 / Å³         | 2315.0(5) |
| Z                   | 2 |
| Density (calculated) / (mg m⁻³) | 1.459 |
| Absorption coefficient / mm⁻¹ | 0.215 |
| F(000)              | 1048 |
| Crystal size / mm³  | 0.380 × 0.300 × 0.160 |
| Theta range for data collection / degree | 3.389-25.350 |
| Index ranges        | −10 ≤ h ≤ 10, −15 ≤ k ≤ 15, −26 ≤ l ≤ 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 F² |
| Data / restraints / parameters | 8467 / 102 / 597 |
| Goodness-of-fit on F² | 1.326 |
| Final R indices [I > 2σ(I)] | R₁ = 0.1001, wR₂ = 0.2620 |
| R indices (all data) | R₁ = 0.1275, wR₂ = 0.2845 |
| Extinction coefficient | n/a |
| Largest diff. peak and hole / e.Å⁻³ | 1.077 and −0.886 |
| Bond          | Length [Å] | Bond          | Length [Å] |
|---------------|------------|---------------|------------|
| 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) 1.390(10) C(41)-F(11P) 1.610(16)
C(25)-F(5) 1.347(12) C(42)-H(42) 0.9500
C(26)-H(26) 0.9500 C(43)-H(43A) 0.9800
C(27)-C(28) 1.391(6) C(43)-H(43B) 0.9800
C(27)-H(27) 0.9500 C(43)-H(43C) 0.9800
C(28)-C(29) 1.387(7) O(1M)-H(1M) 0.8400
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)
| Bond                  | Angle (°)   | Bond                  | Angle (°)   |
|----------------------|------------|----------------------|------------|
| N(2)-C(6)-H(6A)      | 108.7      | C(14)-C(13)-C(12)    | 120.9(4)   |
| C(5)-C(6)-H(6A)      | 108.7      | C(13)-C(14)-C(18)    | 120.2(4)   |
| N(2)-C(6)-H(6B)      | 108.7      | C(13)-C(14)-S(2)     | 118.8(4)   |
| C(5)-C(6)-H(6B)      | 108.7      | C(18)-C(14)-S(2)     | 120.3(3)   |
| H(6A)-C(6)-H(6B)     | 107.6      | O(5)-C(15)-N(4)      | 124.9(6)   |
| O(2)-C(7)-N(3)       | 127.3(5)   | O(5)-C(15)-S(2)      | 121.2(5)   |
| O(2)-C(7)-N(2)       | 126.5(5)   | N(4)-C(15)-S(2)      | 113.9(5)   |
| N(3)-C(7)-N(2)       | 106.1(5)   | N(4)-C(16)-H(16A)    | 109.5      |
| N(3)-C(8)-O(3)       | 105.1(5)   | N(4)-C(16)-H(16B)    | 109.5      |
| N(3)-C(8)-C(10)      | 103.8(5)   | H(16A)-C(16)-H(16B)  | 109.5      |
| O(3)-C(8)-C(10)      | 110.9(5)   | N(4)-C(16)-H(16C)    | 109.5      |
| N(3)-C(8)-H(8)       | 112.2      | H(16A)-C(16)-H(16C)  | 109.5      |
| O(3)-C(8)-H(8)       | 112.2      | H(16B)-C(16)-H(16C)  | 109.5      |
| C(10)-C(8)-H(8)      | 112.2      | N(4)-C(17)-H(17A)    | 109.5      |
| O(3)-C(9)-H(9A)      | 109.5      | N(4)-C(17)-H(17B)    | 109.5      |
| O(3)-C(9)-H(9B)      | 109.5      | H(17A)-C(17)-H(17B)  | 109.5      |
| H(9A)-C(9)-H(9B)     | 109.5      | N(4)-C(17)-H(17C)    | 109.5      |
| O(3)-C(9)-H(9C)      | 109.5      | H(17A)-C(17)-H(17C)  | 109.5      |
| H(9A)-C(9)-H(9C)     | 109.5      | H(17B)-C(17)-H(17C)  | 109.5      |
| H(9B)-C(9)-H(9C)     | 109.5      | C(27)-C(18)-C(14)    | 119.0(4)   |
| O(4)-C(10)-N(2)      | 117.4(5)   | C(27)-C(18)-C(19)    | 117.9(4)   |
| O(4)-C(10)-C(8)      | 107.3(5)   | C(14)-C(18)-C(19)    | 123.0(4)   |
| N(2)-C(10)-C(8)      | 101.7(5)   | C(26)-C(19)-C(20)    | 118.5(4)   |
| O(4)-C(10)-H(10)     | 110.0      | C(26)-C(19)-C(18)    | 119.7(4)   |
| N(2)-C(10)-H(10)     | 110.0      | C(21)-C(20)-C(19)    | 121.8(4)   |
| C(8)-C(10)-H(10)     | 110.0      | C(21)-C(20)-C(19)    | 120.4(4)   |
| O(4)-C(11)-H(11A)    | 109.5      | C(21)-C(20)-H(20)    | 119.8      |
| O(4)-C(11)-H(11B)    | 109.5      | C(19)-C(20)-H(20)    | 119.8      |
| H(11A)-C(11)-H(11B)  | 109.5      | C(23)-C(21)-C(20)    | 120.6(5)   |
| O(4)-C(11)-H(11C)    | 109.5      | C(23)-C(21)-C(22)    | 119.4(4)   |
| H(11A)-C(11)-H(11C)  | 109.5      | C(20)-C(21)-C(22)    | 119.9(5)   |
| H(11B)-C(11)-H(11C)  | 109.5      | F(1P)-C(22)-F(2P)    | 112.1(7)   |
| N(3)-C(12)-C(13)     | 113.5(4)   | F(2)-C(22)-F(3)      | 107.3(6)   |
| N(3)-C(12)-H(12A)    | 108.9      | F(2)-C(22)-F(1)      | 102.9(6)   |
| C(13)-C(12)-H(12A)   | 108.9      | F(3)-C(22)-F(1)      | 102.7(6)   |
| N(3)-C(12)-H(12B)    | 108.9      | F(1P)-C(22)-F(3P)    | 104.6(7)   |
| C(13)-C(12)-H(12B)   | 108.9      | F(2P)-C(22)-F(3P)    | 105.5(6)   |
| H(12A)-C(12)-H(12B)  | 107.7      | F(1P)-C(22)-C(21)    | 112.2(5)   |
| C(29)-C(13)-C(14)    | 118.8(4)   | F(2)-C(22)-C(21)     | 116.5(6)   |
| C(29)-C(13)-C(12)    | 120.2(4)   | F(2P)-C(22)-C(21)    | 113.5(6)   |
| Bond          | Angle (°)  |
|--------------|-----------|
| 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(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     |
| 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) | 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)  | 110.6(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)  |
| Bond/Angle | Value |
|-----------|-------|
| 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 Å   Wavelength=0.71073 Å

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

Temperature:  130 K

Volume  952.5(6) Å³  952.6(6) Å³
Space group  P -1  P -1
Hall group  -P 1  -P 1
Moiety formula  C19 H17 F6 N O2 S  C19 H17 F6 N O2
S1 Sum formula  C19 H17 F6 N O2 S  C19 H17 F6 N O2
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  Θ(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
Low Bond Precision on C-C Bonds ............ 0.005 Ang.

Alert level G
Number of Distance or Angle Restraints on AtSite 2
Note No Embedded Refinement Details Found in the CIF Please Do ! Low 'MainMol' Ueq as Compared to Neighbors of C7 Check Low 'MainMol' Ueq as Compared to Neighbors of C8 Check Number of Least-Squares Restraints ............ 1

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
5 ALERT level G = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
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.

1 ALERT level A = Data missing that is essential or data in wrong format
0 ALERT level G = General alerts. Data that may be required is missing

Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements.

However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

# 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
**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.  

**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                         |                  |

| 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         |
| Dxm, 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

The value of Rint is greater than 0.12

Rint given 0.137

The Value of Rint is Greater Than 0.12 .......... 0.137 Report

Atom F2 has ADP max/min Ratio ...... 3.1 prolat
Atom F3 has ADP max/min Ratio ...... 3.1 prolat

Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.1 Ratio

Large Hirshfeld Difference F10 -- C38 0.19 Ang.
Single Bonded Oxygen (C-O > 1.3 Ang) ............... 0IP Check
Low Bond Precision on C-C Bonds ............ 0.01114 Ang.

Long H...A H-Bond Reported H4B ..I1 3.09 Ang.
Long H...A H-Bond Reported H21B ..F2 2.65 Ang.
Long H...A H-Bond Reported H22B ..I1 3.09 Ang.

Alert level G

No Embedded Refinement Details Foundin the CIF Please Do !

SHELXL Second Parameter in WGH T Unusually Large 68.88

Why ? Hirshfeld Test Diff for F12P --C38 ..
7.8 s.u. Hirshfeld Test Diff forF12P --C38 ..
6.7 s.u. Hirshfeld Test

Diff for F12 --C38 .. 6.6

s.u. Low 'MainMol' Ueq as Compared to Neighbors of
C18 Check Low 'MainMol' Ueq as Compared to Neighbors of
C19 Check Low '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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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
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PLAT205_ALERT_3_C
PLAT213_ALERT_2_C
PLAT213_ALERT_2_C
PLAT220_ALERT_2_C
PLAT234_ALERT_4_C
PLAT309_ALERT_2_C
PLAT301_ALERT_3_G
PLAT234_ALERT_4_C
PLAT242_ALERT_2_G
PLAT301_ALERT_3_G
PLAT342_ALERT_3_C
PLAT480_ALERT_4_C
PLAT480_ALERT_4_C
PLAT480_ALERT_4_C
PLAT005_ALERT_5_G
PLAT083_ALERT_2_G
PLAT230_ALERT_2_G
PLAT230_ALERT_2_G
PLAT230_ALERT_2_G
PLAT242_ALERT_2_G
PLAT242_ALERT_2_G
PLAT242_ALERT_2_G
PLAT301_ALERT_3_G
PLAT434_ALERT_2_G
PLAT790_ALERT_4_G

Alert level A

PUBL012_ALERT_1_A_publ_section_abstract is missing.
Abstract of paper in English.

3 ALERT level A = Data missing that is essential or data in wrong format
0 ALERT level G = General alerts. Data that may be required is missing
**Publication of your CIF**

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**Validation response form**

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```plaintext
# 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.

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

**Datablock: I**

| Bond precision: | C-C = 0.0070 Å | 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          |                    |
| Volume          | Calculated     | Reported           |
|                 | 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,l max       | 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
\[\text{test-name}_\text{_ALERT}_\text{_alert-type}_\text{_alert-level}\]
Click on the hyperlinks for more details of the test.

**Alert level C**

PLAT048_ALERT_1_C
PLAT084_ALERT_3_C
PLAT220_ALERT_2_C
PLAT222_ALERT_3_C
PLAT242_ALERT_2_C
PLAT340_ALERT_3_C

Alert level G

PLAT003_ALERT_2_G
PLAT005_ALERT_5_G
PLAT007_ALERT_5_G
PLAT072_ALERT_2_G
PLAT230_ALERT_2_G
PLAT230_ALERT_2_G
PLAT230_ALERT_2_G
PLAT230_ALERT_2_G
PLAT230_ALERT_2_G
PLAT230_ALERT_2_G
PLAT230_ALERT_2_G
PLAT230_ALERT_2_G
PLAT230_ALERT_2_G
PLAT242_ALERT_2_G
PLAT242_ALERT_2_G
PLAT301_ALERT_3_G
PLAT432_ALERT_2_G
PLAT720_ALERT_4_G
PLAT790_ALERT_4_G

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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2 ALERT type 5 Informative message, check

checkCIF publication errors
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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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