# Mesomorphic and Ion Conducting Properties of Dialkyl(1,4-phenylene)diimidazolium Salts

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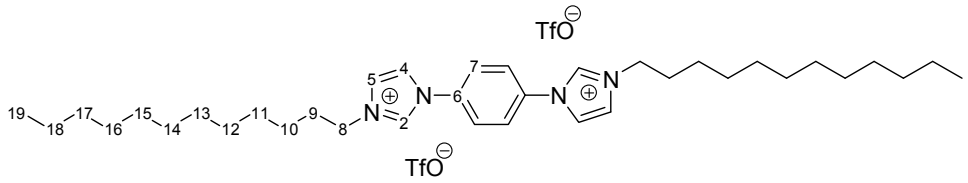
# Supporting Information:


TfO
TfO
N
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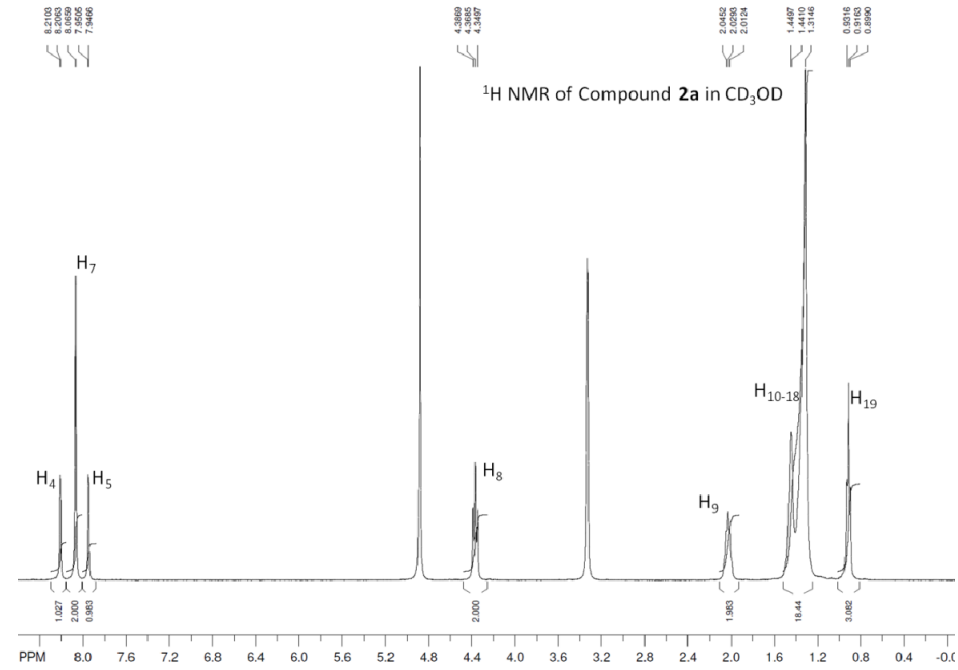
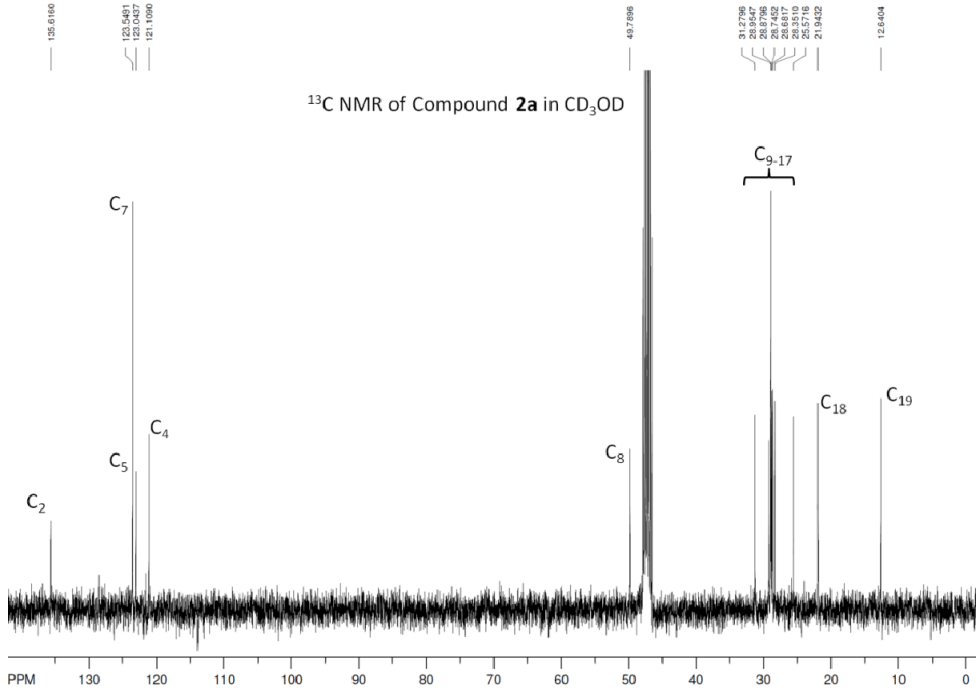
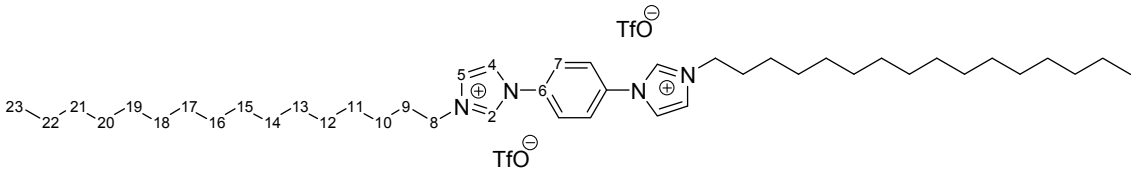
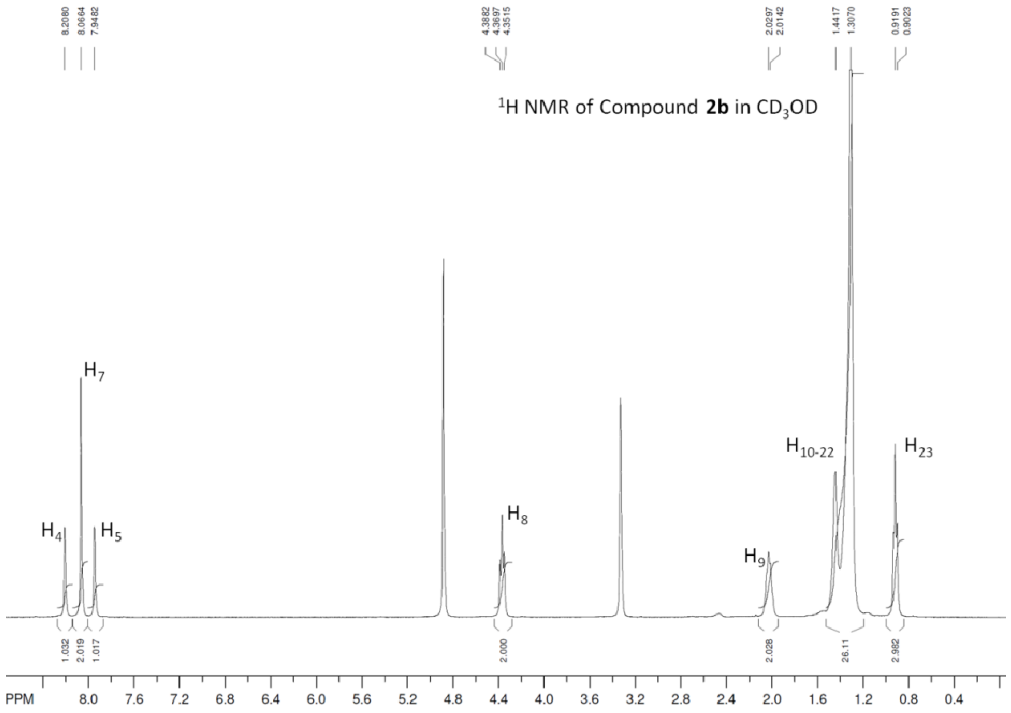
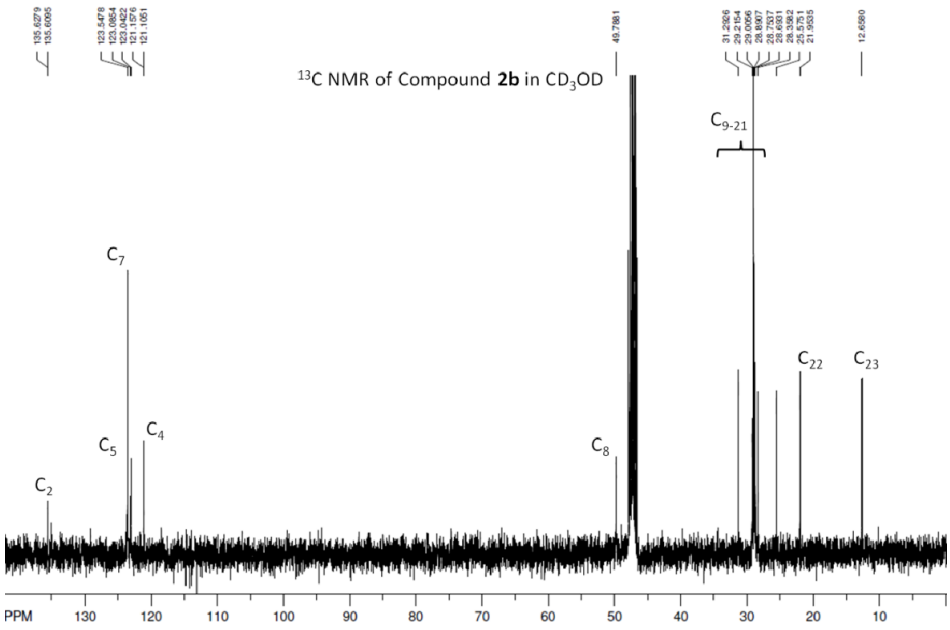
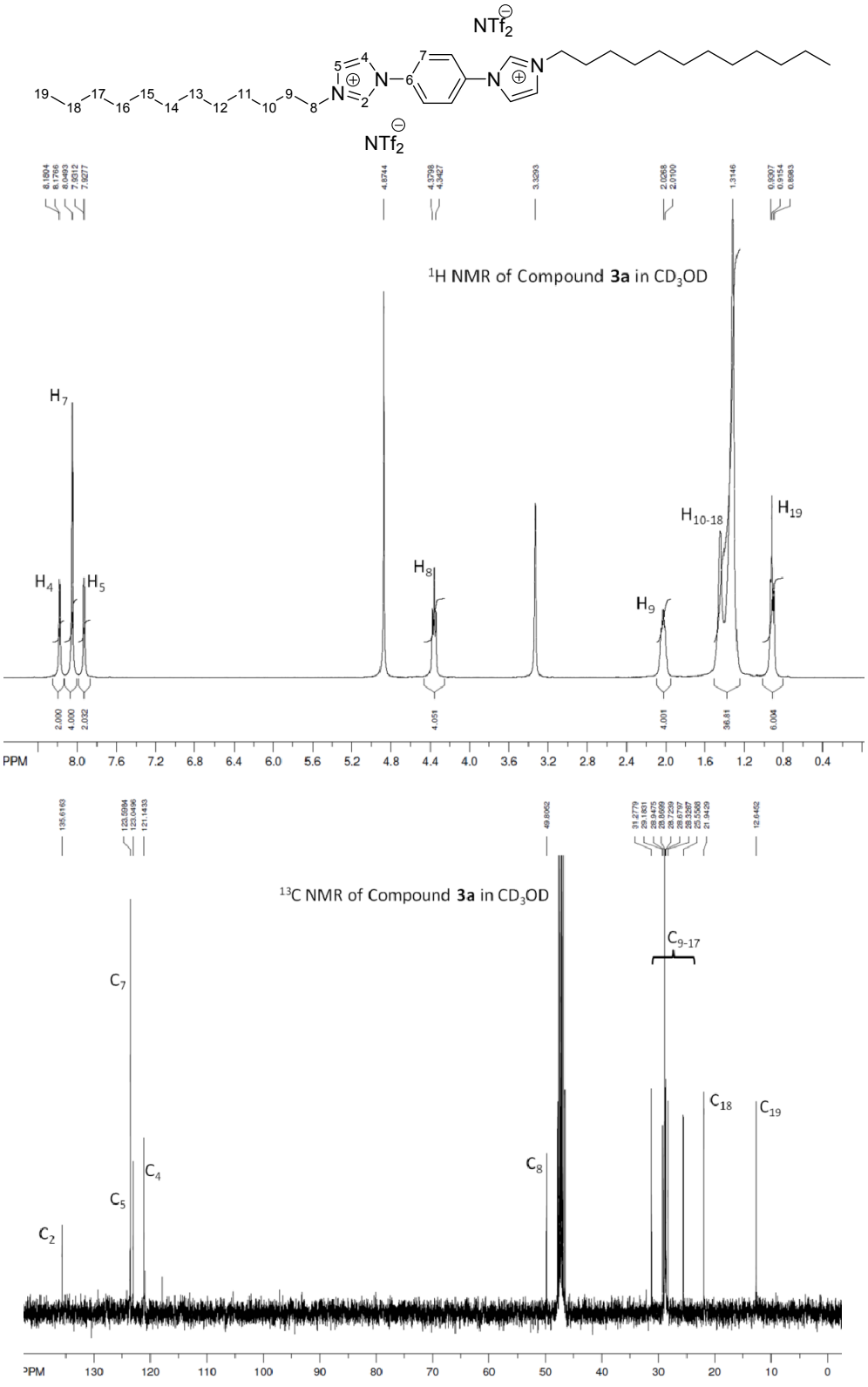

$^1$H NMR of Compound **2a** in $CD_3OD$
$H_4$
$H_5$
$H_7$
$H_8$
$H_9$
$H_{10-18}$
$H_{19}$
PPM

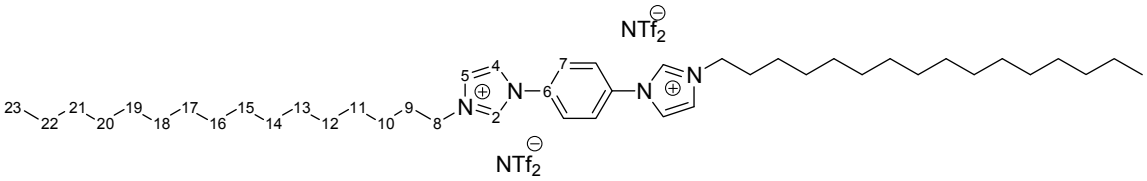

$^{13}$C NMR of Compound **2a** in $CD_3OD$
$C_2$
$C_4$
$C_5$
$C_7$
$C_8$
$C_{9-17}$
$C_{18}$
$C_{19}$
PPM

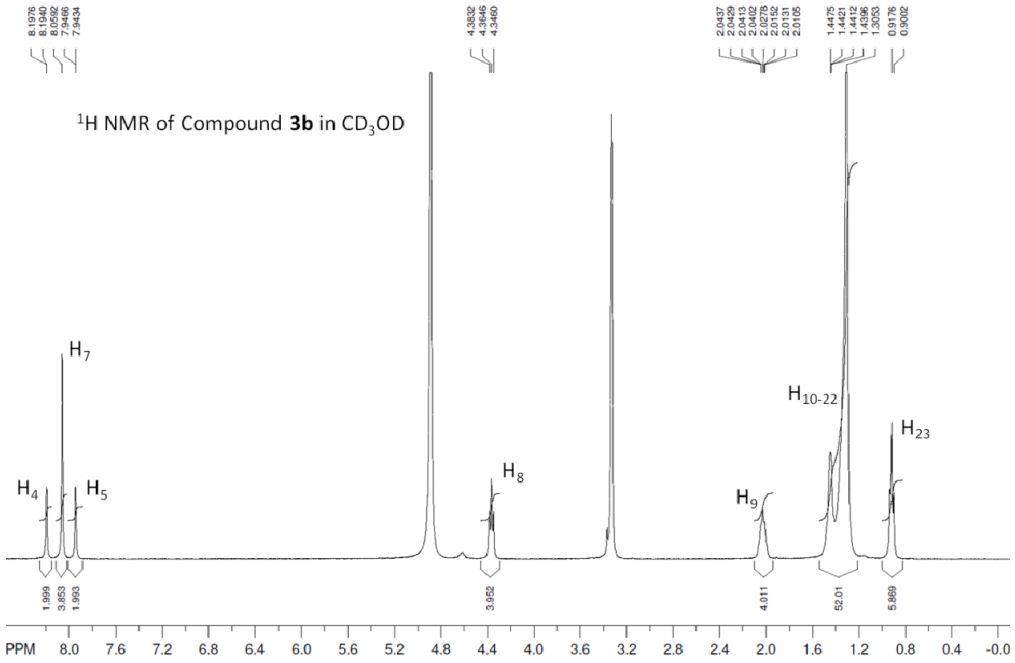

TfO
TfO

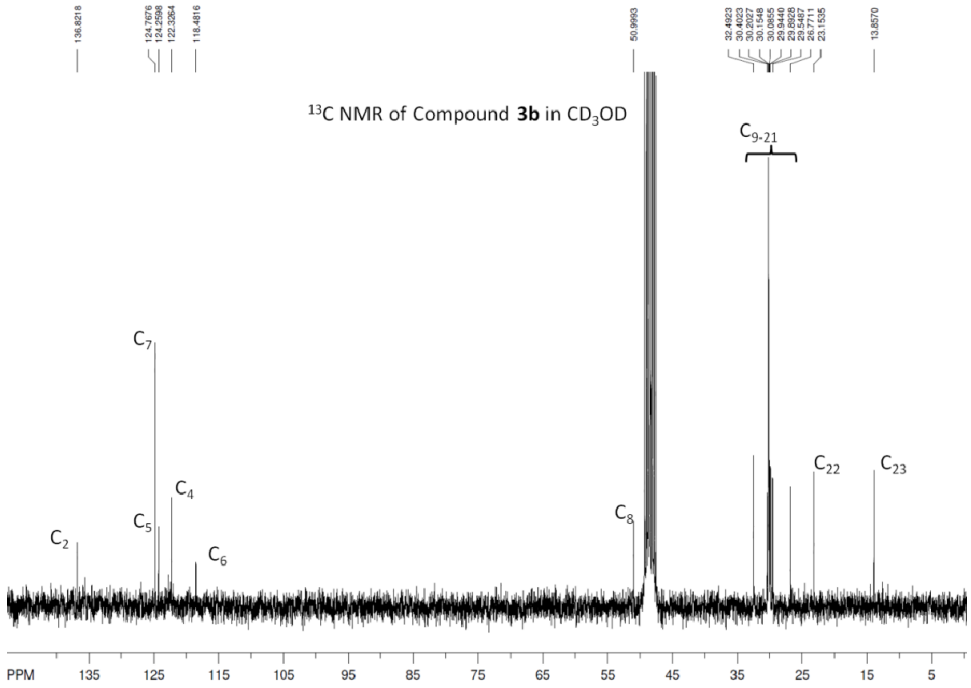

$^1$H NMR of Compound **2b** in $CD_3OD$
H7
H4
H5
H8
H9
H10-22
H23
PPM


$^{13}$C NMR of Compound **2b** in $CD_3OD$
C9-21
C7
C5
C4
C2
C8
C22
C23
PPM

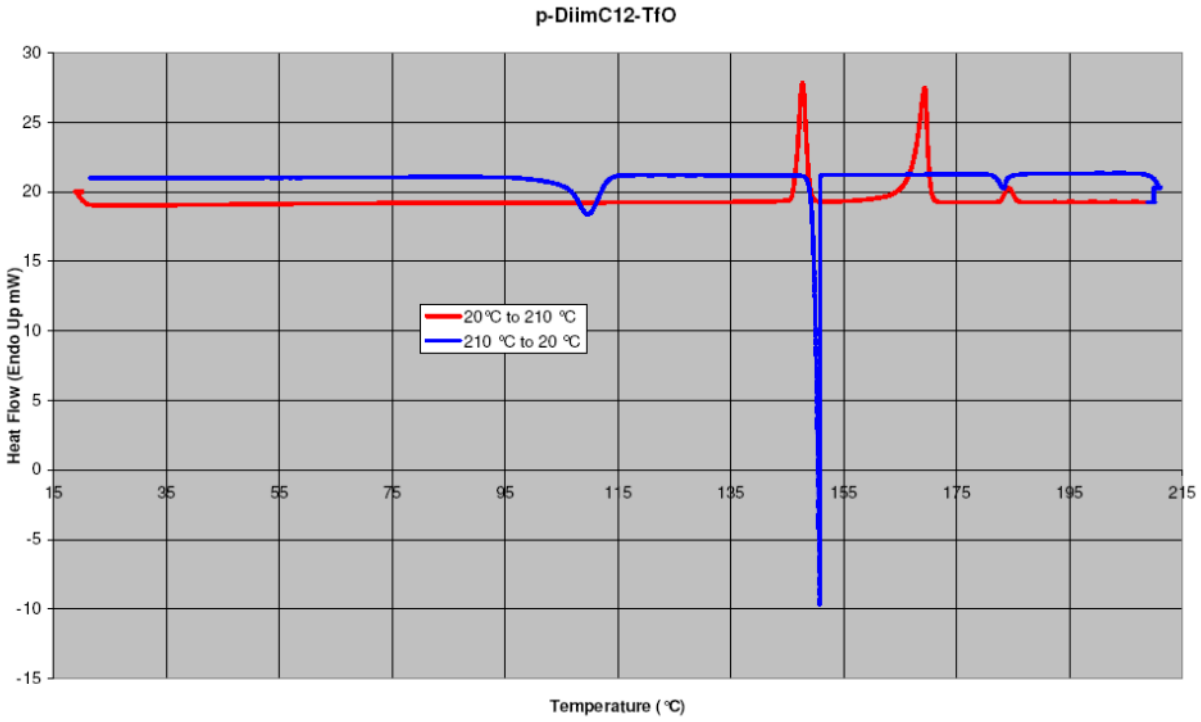

NTf2
NTf2
1H NMR of Compound 3a in CD3OD
H7
H4
H5
H8
H9
H10-18
H19
PPM
13C NMR of Compound 3a in CD3OD
C7
C4
C5
C2
C8
C9-17
C18
C19
PPM


NTf2
NTf2

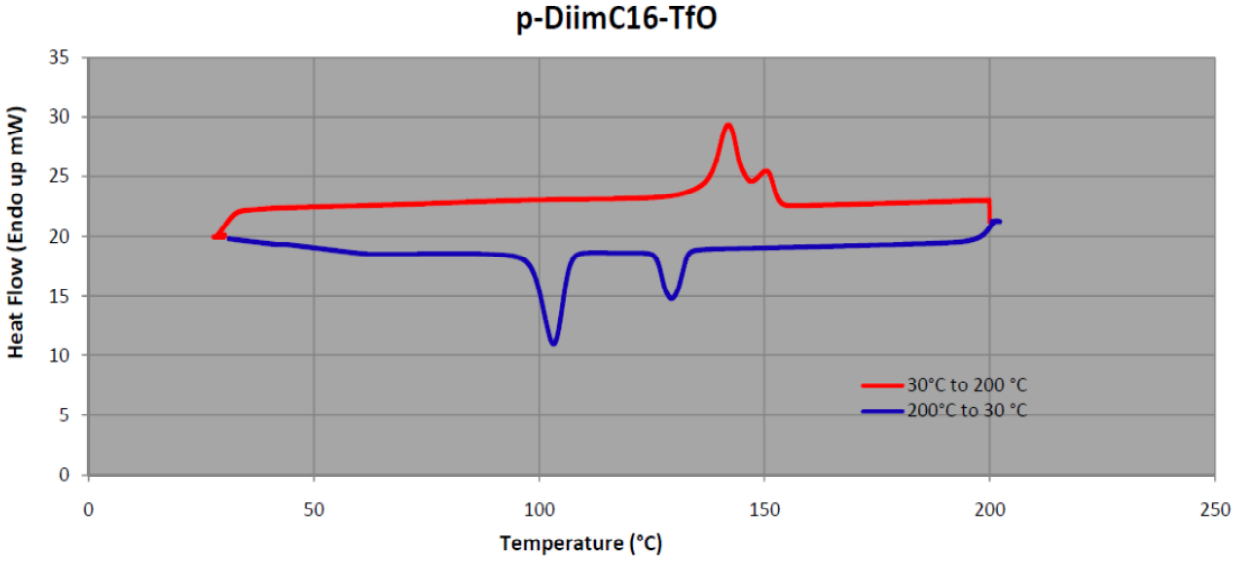

1H NMR of Compound 3b in CD3OD
H7
H4
H5
H8
H9
H10-22
H23
PPM


13C NMR of Compound 3b in CD3OD
C9-21
C7
C4
C5
C2
C6
C8
C22
C23
PPM

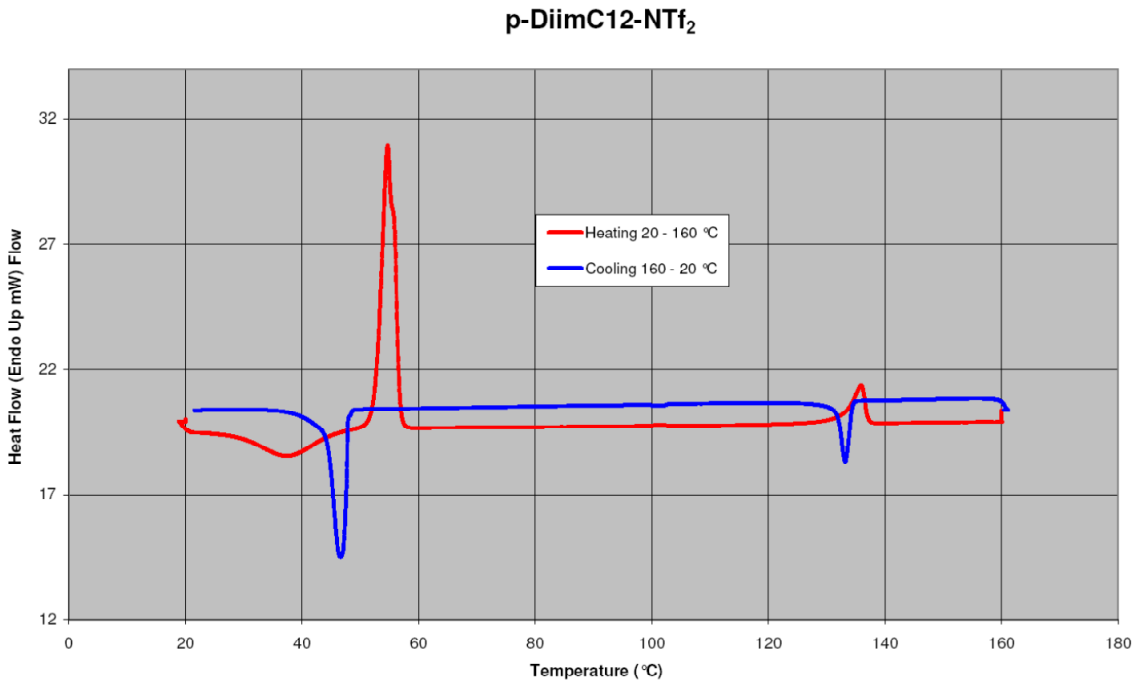
DSC of compound **2a:** (first and second cycles (heating+cooling) identical)



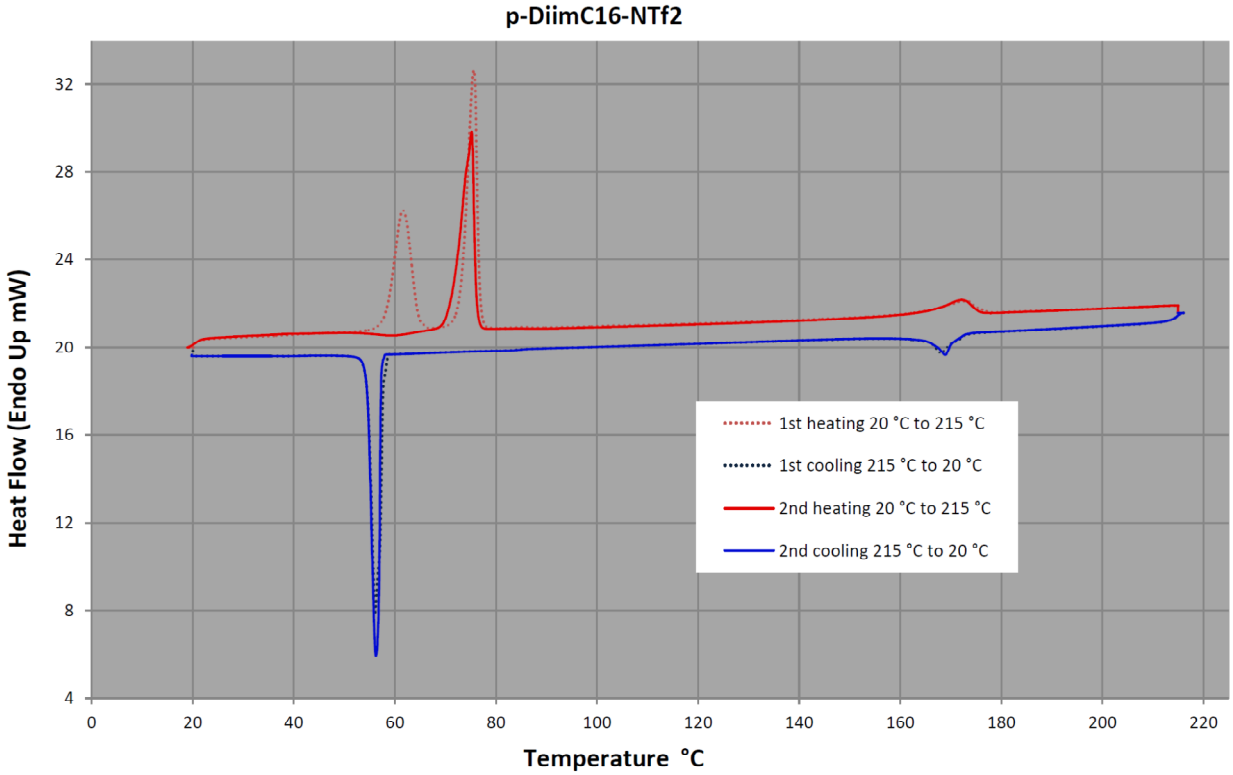

DSC of compound **2b:** (first and second cycles identical)



DSC of compound **3a:** (first and second cycles identical)

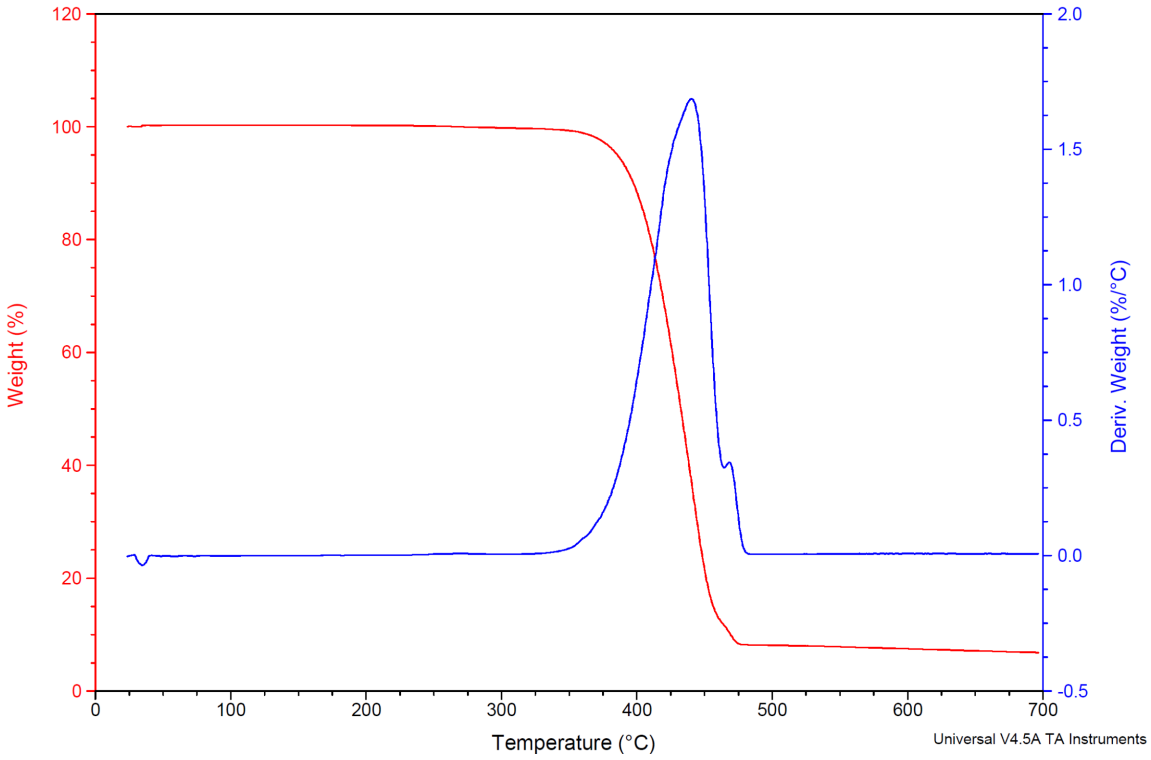



DSC of compound **3b:**

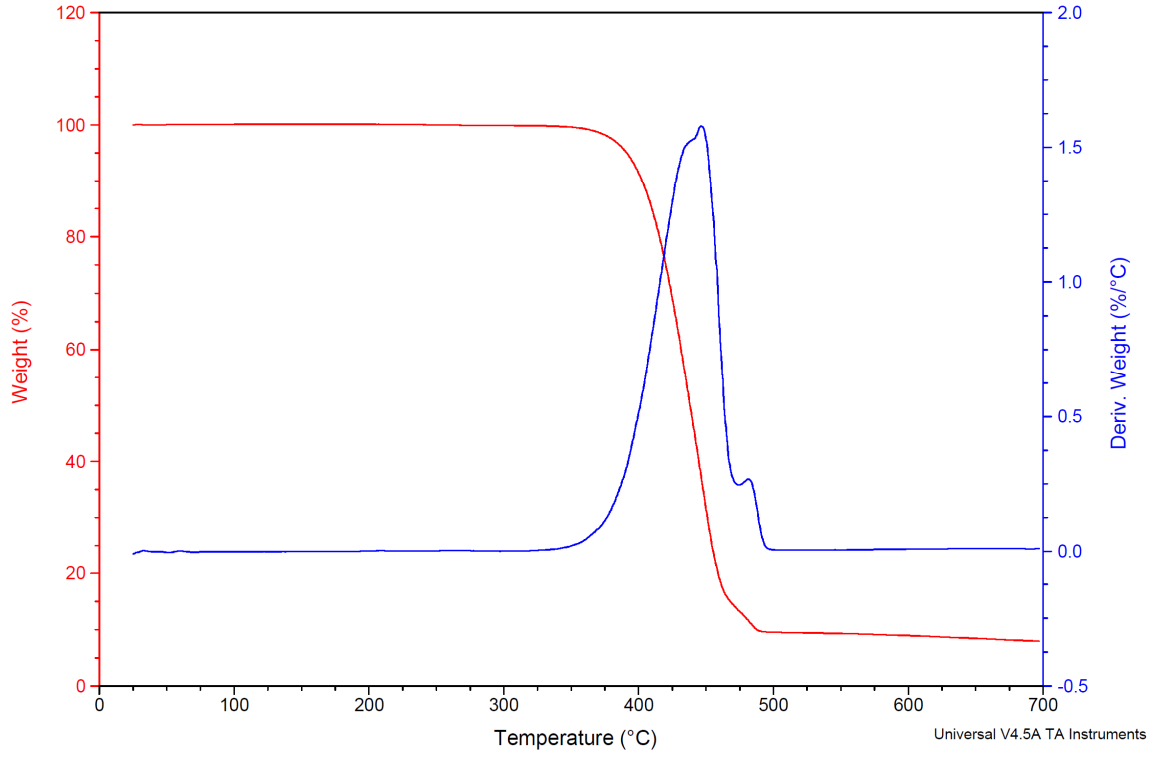



The first heating shows a phase transition at 60 °C that isn't present in the subsequent heating cycles. This is due to the crystallization of compound 3b in different crystalline phases upon synthesis or upon cooling from the Smectic phase.

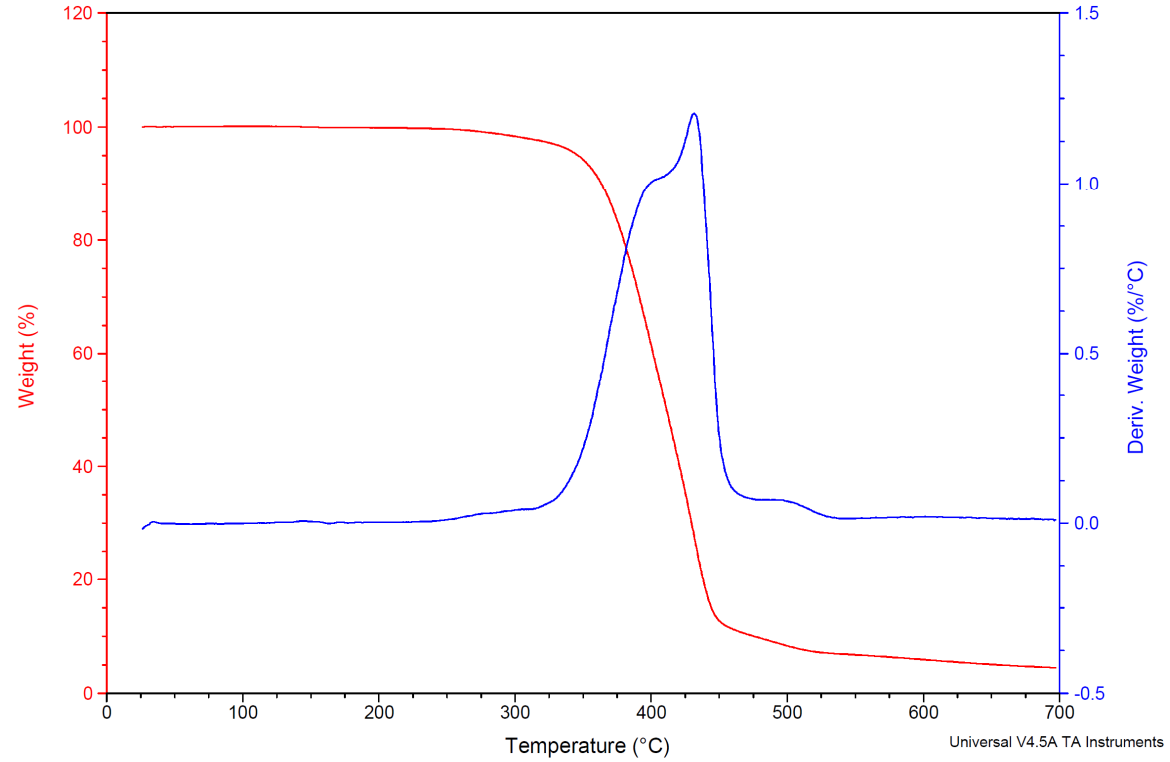
TGA of compound **2a:**



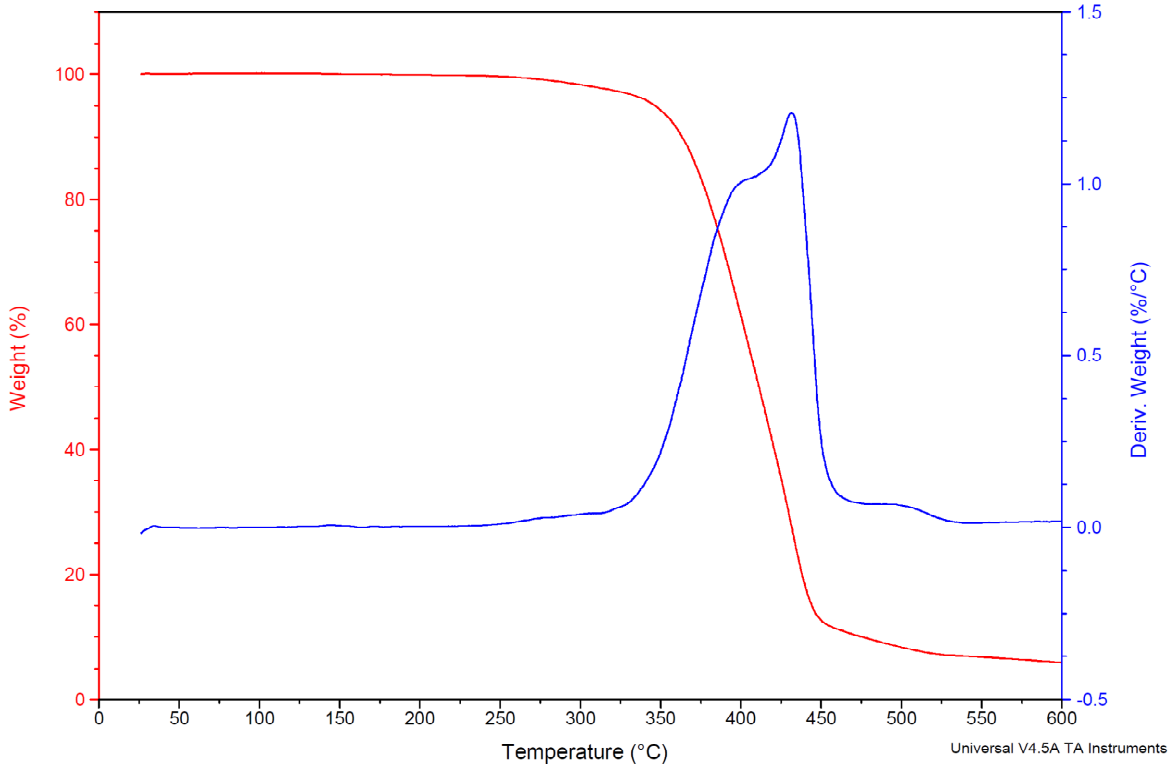

TGA of compound **2b:**



TGA of compound **3a:**




TGA of compound **3b:**



# Crystallographic data for compound 2a.

**CRYSTAL AND MOLECULAR STRUCTURE OF**

**C38 H60 F6 N4 O6 S2 COMPOUND 2a**

Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Nadim Noujeim.

**Table 1.** Crystal data and structure refinement for C38 H60 F6 N4 O6 S2.

| | |
|---|---|
| Identification code | NADIM2 |
| Empirical formula | C38 H60 F6 N4 O6 S2 |
| Formula weight | 847.02 |
| Temperature | 150K |
| Wavelength | 1.54178 Å |
| Crystal system | Triclinic |
| Space group | P-1 |
| Unit cell dimensions | a = 8.4599(2) Å α = 81.9423(11)°<br>b = 8.5465(2) Å β = 76.9685(11)°<br>c = 16.5655(4) Å γ = 72.9996(10)° |
| Volume | 1112.34(5)Å$^3$ |
| Z | 1 |
| Density (calculated) | 1.264 g/cm$^3$ |
| Absorption coefficient | 1.699 mm$^{-1}$ |
| F(000) | 450 |
| Crystal size | 0.26 x 0.24 x 0.07 mm |
| Theta range for data collection | 2.75 to 72.55° |
| Index ranges | $-10 \le h \le 10$, $-9 \le k \le 10$, $-20 \le \ell \le 20$ |
| Reflections collected | 29749 |
| Independent reflections | 4288 [$R_{int}$ = 0.038] |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.8879 and 0.7721 |
| Refinement method | Full-matrix least-squares on F$^2$ |
| Data / restraints / parameters | 4288 / 0 / 255 |
| Goodness-of-fit on F$^2$ | 1.031 |
| Final R indices [I>2sigma(I)] | $R_1$ = 0.0430, $wR_2$ = 0.1151 |
| R indices (all data) | $R_1$ = 0.0443, $wR_2$ = 0.1163 |
| Extinction coefficient | 0.0125(9) |

| | |
|---|---|
| Largest diff. peak and hole | 0.324 and -0.419 e/Å$^3$ |

**Table 2.** Atomic coordinates (x $10^4$) and equivalent isotropic displacement parameters (Å$^2$ x $10^3$) for C38 H60 F6 N4 O6 S2.

$U_{eq}$ is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| N(1) | 6925(2) | 8841(1) | 1195(1) | 29(1) |
| C(2) | 5837(2) | 8320(2) | 912(1) | 28(1) |
| N(3) | 6476(1) | 6715(1) | 810(1) | 27(1) |
| C(4) | 8038(2) | 6200(2) | 1039(1) | 30(1) |
| C(5) | 8316(2) | 7532(2) | 1281(1) | 32(1) |
| C(6) | 5720(2) | 5812(2) | 409(1) | 26(1) |
| C(7) | 3977(2) | 6209(2) | 519(1) | 28(1) |
| C(8) | 6754(2) | 4611(2) | -104(1) | 29(1) |
| C(9) | 6700(2) | 10589(2) | 1298(1) | 33(1) |
| C(10) | 6250(2) | 10999(2) | 2196(1) | 32(1) |
| C(11) | 5713(2) | 12866(2) | 2219(1) | 32(1) |
| C(12) | 5193(2) | 13466(2) | 3087(1) | 38(1) |
| C(13) | 4650(2) | 15335(2) | 3073(1) | 39(1) |
| C(14) | 4159(2) | 15973(2) | 3933(1) | 43(1) |
| C(15) | 3536(2) | 17839(2) | 3919(1) | 43(1) |
| C(16) | 3083(2) | 18481(2) | 4779(1) | 44(1) |
| C(17) | 2401(3) | 20341(2) | 4765(1) | 45(1) |
| C(18) | 1966(3) | 21008(2) | 5615(1) | 47(1) |
| C(19) | 1259(3) | 22857(2) | 5591(1) | 61(1) |
| C(20) | 829(4) | 23524(3) | 6443(2) | 81(1) |
| S(25) | 1170(1) | 1240(1) | 1238(1) | 31(1) |
| O(26) | -149(1) | 2366(1) | 863(1) | 39(1) |
| O(27) | 2853(1) | 1251(1) | 810(1) | 45(1) |
| O(28) | 944(2) | -367(1) | 1507(1) | 48(1) |
| C(21) | 971(2) | 2154(2) | 2201(1) | 41(1) |
| F(22) | 2133(2) | 1295(2) | 2631(1) | 67(1) |
| F(23) | -527(2) | 2258(2) | 2688(1) | 67(1) |
| F(24) | 1159(2) | 3674(1) | 2036(1) | 61(1) |

**Table 3.** Hydrogen coordinates (x $10^4$) and isotropic displacement parameters (Å$^2$ x $10^3$) for C38 H60 F6 N4 O6 S2.

| | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| H(2) | 4779 | 8976 | 801 | 34 |
| H(4) | 8773 | 5120 | 1028 | 36 |
| H(5) | 9282 | 7561 | 1474 | 39 |
| H(7) | 3291 | 7034 | 874 | 34 |
| H(8) | 7945 | 4354 | -171 | 34 |
| H(9A) | 5799 | 11270 | 1007 | 39 |
| H(9B) | 7756 | 10883 | 1029 | 39 |
| H(10A) | 7236 | 10516 | 2465 | 39 |
| H(10B) | 5319 | 10536 | 2501 | 39 |
| H(11A) | 6660 | 13302 | 1909 | 39 |
| H(11B) | 4757 | 13325 | 1927 | 39 |
| H(12A) | 6151 | 13031 | 3380 | 45 |
| H(12B) | 4250 | 13031 | 3403 | 45 |
| H(13A) | 5586 | 15767 | 2744 | 47 |
| H(13B) | 3679 | 15764 | 2789 | 47 |
| H(14A) | 5147 | 15590 | 4206 | 52 |
| H(14B) | 3261 | 15498 | 4272 | 52 |
| H(15A) | 2531 | 18219 | 3658 | 52 |
| H(15B) | 4423 | 18314 | 3569 | 52 |
| H(16A) | 2226 | 17974 | 5135 | 53 |
| H(16B) | 4099 | 18137 | 5031 | 53 |
| H(17A) | 3252 | 20845 | 4400 | 54 |
| H(17B) | 1378 | 20680 | 4518 | 54 |
| H(18A) | 1130 | 20493 | 5984 | 56 |
| H(18B) | 2994 | 20692 | 5857 | 56 |
| H(19A) | 228 | 23174 | 5351 | 74 |
| H(19B) | 2093 | 23374 | 5220 | 74 |
| H(20A) | -30 | 23053 | 6808 | 121 |
| H(20B) | 396 | 24722 | 6385 | 121 |
| H(20C) | 1845 | 23225 | 6684 | 121 |

**Table 4.** Anisotropic parameters ($Å^2$ x $10^3$) for C38 H60 F6 N4 O6 S2.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [ h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12} ]$$

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| N(1) | 37(1) | 22(1) | 30(1) | -4(1) | -9(1) | -7(1) |
| C(2) | 35(1) | 20(1) | 30(1) | -4(1) | -9(1) | -5(1) |
| N(3) | 31(1) | 20(1) | 28(1) | -3(1) | -8(1) | -5(1) |
| C(4) | 32(1) | 25(1) | 34(1) | -3(1) | -9(1) | -4(1) |
| C(5) | 34(1) | 28(1) | 36(1) | -3(1) | -11(1) | -7(1) |
| C(6) | 34(1) | 18(1) | 26(1) | -1(1) | -9(1) | -6(1) |
| C(7) | 33(1) | 21(1) | 29(1) | -6(1) | -5(1) | -3(1) |
| C(8) | 29(1) | 24(1) | 32(1) | -3(1) | -7(1) | -4(1) |
| C(9) | 46(1) | 20(1) | 34(1) | -3(1) | -11(1) | -11(1) |
| C(10) | 41(1) | 23(1) | 32(1) | -4(1) | -7(1) | -7(1) |
| C(11) | 40(1) | 23(1) | 33(1) | -3(1) | -5(1) | -7(1) |
| C(12) | 51(1) | 25(1) | 32(1) | -5(1) | -1(1) | -8(1) |
| C(13) | 54(1) | 26(1) | 33(1) | -5(1) | -2(1) | -8(1) |
| C(14) | 63(1) | 27(1) | 33(1) | -5(1) | 1(1) | -8(1) |
| C(15) | 65(1) | 27(1) | 32(1) | -6(1) | -2(1) | -9(1) |
| C(16) | 66(1) | 29(1) | 32(1) | -6(1) | -2(1) | -10(1) |
| C(17) | 69(1) | 30(1) | 33(1) | -7(1) | -3(1) | -11(1) |
| C(18) | 66(1) | 37(1) | 35(1) | -11(1) | -2(1) | -13(1) |
| C(19) | 90(2) | 39(1) | 51(1) | -19(1) | -5(1) | -11(1) |
| C(20) | 108(2) | 63(2) | 69(2) | -41(1) | -4(1) | -15(1) |
| S(25) | 33(1) | 22(1) | 34(1) | -3(1) | -5(1) | -1(1) |
| O(26) | 43(1) | 31(1) | 41(1) | -5(1) | -16(1) | 2(1) |
| O(27) | 37(1) | 38(1) | 48(1) | 0(1) | 3(1) | -1(1) |
| O(28) | 56(1) | 26(1) | 62(1) | 1(1) | -13(1) | -12(1) |
| C(21) | 37(1) | 47(1) | 38(1) | -4(1) | -10(1) | -9(1) |
| F(22) | 64(1) | 84(1) | 54(1) | 5(1) | -34(1) | -13(1) |
| F(23) | 51(1) | 106(1) | 45(1) | -28(1) | 6(1) | -24(1) |
| F(24) | 75(1) | 46(1) | 70(1) | -20(1) | -19(1) | -18(1) |

**Table 5.** Bond lengths [Å] and angles [°] for C38 H60 F6 N4 O6 S2

| | | | |
|---|---|---|---|
| N(1)-C(2) | 1.3255(18) | C(2)-N(3)-C(4) | 108.49(11) |
| N(1)-C(5) | 1.3844(18) | C(2)-N(3)-C(6) | 123.02(11) |
| N(1)-C(9) | 1.4791(17) | C(4)-N(3)-C(6) | 127.88(11) |
| C(2)-N(3) | 1.3384(17) | C(5)-C(4)-N(3) | 106.87(12) |
| N(3)-C(4) | 1.3861(17) | C(4)-C(5)-N(1) | 107.05(12) |
| N(3)-C(6) | 1.4384(17) | C(7)-C(6)-C(8) | 121.65(13) |
| C(4)-C(5) | 1.357(2) | C(7)-C(6)-N(3) | 119.18(12) |
| C(6)-C(7) | 1.3883(19) | C(8)-C(6)-N(3) | 119.11(12) |
| C(6)-C(8) | 1.3883(19) | C(8)#1-C(7)-C(6) | 119.31(13) |
| C(7)-C(8)#1 | 1.3879(19) | C(7)#1-C(8)-C(6) | 119.03(13) |
| C(8)-C(7)#1 | 1.3879(19) | N(1)-C(9)-C(10) | 113.82(11) |
| C(9)-C(10) | 1.515(2) | C(9)-C(10)-C(11) | 108.73(11) |
| C(10)-C(11) | 1.5296(19) | C(12)-C(11)-C(10) | 114.75(12) |
| C(11)-C(12) | 1.521(2) | C(11)-C(12)-C(13) | 112.47(12) |
| C(12)-C(13) | 1.526(2) | C(14)-C(13)-C(12) | 113.66(12) |
| C(13)-C(14) | 1.522(2) | C(13)-C(14)-C(15) | 113.53(13) |
| C(14)-C(15) | 1.525(2) | C(14)-C(15)-C(16) | 113.58(13) |
| C(15)-C(16) | 1.525(2) | C(17)-C(16)-C(15) | 113.41(13) |
| C(16)-C(17) | 1.523(2) | C(18)-C(17)-C(16) | 114.23(14) |
| C(17)-C(18) | 1.520(2) | C(19)-C(18)-C(17) | 113.51(15) |
| C(18)-C(19) | 1.516(3) | C(18)-C(19)-C(20) | 113.42(19) |
| C(19)-C(20) | 1.524(3) | O(28)-S(25)-O(26) | 115.61(7) |
| S(25)-O(28) | 1.4378(11) | O(28)-S(25)-O(27) | 114.60(7) |
| S(25)-O(26) | 1.4403(10) | O(26)-S(25)-O(27) | 114.45(7) |
| S(25)-O(27) | 1.4418(12) | O(28)-S(25)-C(21) | 104.36(8) |
| S(25)-C(21) | 1.8260(17) | O(26)-S(25)-C(21) | 102.84(7) |
| C(21)-F(23) | 1.325(2) | O(27)-S(25)-C(21) | 102.63(8) |
| C(21)-F(22) | 1.3264(19) | F(23)-C(21)-F(22) | 107.82(14) |
| C(21)-F(24) | 1.337(2) | F(23)-C(21)-F(24) | 107.50(15) |
| | | F(22)-C(21)-F(24) | 107.41(14) |
| C(2)-N(1)-C(5) | 108.87(11) | F(23)-C(21)-S(25) | 111.75(11) |
| C(2)-N(1)-C(9) | 123.09(12) | F(22)-C(21)-S(25) | 111.74(12) |
| C(5)-N(1)-C(9) | 127.71(12) | F(24)-C(21)-S(25) | 110.42(11) |
| N(1)-C(2)-N(3) | 108.72(12) | | |

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

**Table 6.** Torsion angles [°] for C38 H60 F6 N4 O6 S2.

| | |
|---|---|
| C(5)-N(1)-C(2)-N(3) | -0.15(16) |
| C(9)-N(1)-C(2)-N(3) | 173.66(12) |
| N(1)-C(2)-N(3)-C(4) | 0.03(15) |
| N(1)-C(2)-N(3)-C(6) | -171.60(12) |
| C(2)-N(3)-C(4)-C(5) | 0.10(16) |
| C(6)-N(3)-C(4)-C(5) | 171.21(13) |
| N(3)-C(4)-C(5)-N(1) | -0.19(16) |
| C(2)-N(1)-C(5)-C(4) | 0.22(16) |
| C(9)-N(1)-C(5)-C(4) | -173.23(13) |
| C(2)-N(3)-C(6)-C(7) | -35.55(19) |
| C(4)-N(3)-C(6)-C(7) | 154.52(13) |
| C(2)-N(3)-C(6)-C(8) | 141.83(13) |
| C(4)-N(3)-C(6)-C(8) | -28.1(2) |
| C(8)-C(6)-C(7)-C(8)#1 | -0.1(2) |
| N(3)-C(6)-C(7)-C(8)#1 | 177.18(11) |
| C(7)-C(6)-C(8)-C(7)#1 | 0.1(2) |
| N(3)-C(6)-C(8)-C(7)#1 | -177.19(11) |
| C(2)-N(1)-C(9)-C(10) | 108.54(15) |
| C(5)-N(1)-C(9)-C(10) | -78.87(18) |
| N(1)-C(9)-C(10)-C(11) | -168.93(12) |
| C(9)-C(10)-C(11)-C(12) | 179.02(13) |
| C(10)-C(11)-C(12)-C(13) | -179.29(13) |
| C(11)-C(12)-C(13)-C(14) | -178.73(14) |
| C(12)-C(13)-C(14)-C(15) | -177.23(15) |
| C(13)-C(14)-C(15)-C(16) | -178.63(15) |
| C(14)-C(15)-C(16)-C(17) | -177.89(16) |
| C(15)-C(16)-C(17)-C(18) | -179.14(16) |
| C(16)-C(17)-C(18)-C(19) | -178.89(18) |
| C(17)-C(18)-C(19)-C(20) | -179.8(2) |
| O(28)-S(25)-C(21)-F(23) | -60.38(14) |
| O(26)-S(25)-C(21)-F(23) | 60.68(14) |
| O(27)-S(25)-C(21)-F(23) | 179.76(12) |
| O(28)-S(25)-C(21)-F(22) | 60.53(14) |
| O(26)-S(25)-C(21)-F(22) | -178.40(12) |
| O(27)-S(25)-C(21)-F(22) | -59.32(13) |
| O(28)-S(25)-C(21)-F(24) | -179.98(11) |
| O(26)-S(25)-C(21)-F(24) | -58.92(13) |
| O(27)-S(25)-C(21)-F(24) | 60.17(12) |

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

**Table 7.** Bond lengths [Å] and angles [°] related to the hydrogen bonding for C38 H60 F6 N4 O6 S2.

| D-H | ..A | d(D-H) | d(H..A) | d(D..A) | <DHA |
|---|---|---|---|---|---|
| C(2)-H(2) | O(27)#2 | 0.95 | 2.14 | 3.0094(18) | 151.5 |

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z  #2 x,y+1,z

# Crystallographic data for compound 3a.

**CRYSTAL AND MOLECULAR STRUCTURE OF**

**C40 H60 F2 N6 O8 S4 COMPOUND (SCHM48)**

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Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Michel Simard.

**Table 1.** Crystal data and structure refinement for C40 H60 $F^2$ N6 O8 S4.

| | |
|---|---|
| Identification code | SCHM48 |
| Empirical formula | C40 H60 F12 N6 O8 S4 |
| Formula weight | 1109.18 |
| Temperature | 200K |
| Wavelength | 1.54178 Å |
| Crystal system | Triclinic |
| Space group | P-1 |
| Unit cell dimensions | a = 5.8927(2) Å α = 80.782(1)°<br>b = 8.7710(2) Å β = 85.616(1)°<br>c = 25.3158(7) Å γ = 79.496(1)° |
| Volume | 1268.40(6)$Å^3$ |
| Z | 1 |
| Density (calculated) | 1.452 $g/cm^3$ |
| Absorption coefficient | 2.599 $mm^{-1}$ |
| F(000) | 578 |
| Crystal size | 0.15 x 0.15 x 0.11 mm |
| Theta range for data collection | 1.77 to 72.56° |
| Index ranges | $-7 \le h \le 7$, $-10 \le k \le 10$, $-31 \le \ell \le 31$ |
| Reflections collected | 32251 |
| Independent reflections | 4869 [$R_{int}$ = 0.036] |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.7513 and 0.5553 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4869 / 118 / 428 |
| Goodness-of-fit on F^2 | 1.056 |
| Final R indices [I>2sigma(I)] | $R_1$ = 0.0374, $wR_2$ = 0.1054 |
| R indices (all data) | $R_1$ = 0.0387, $wR_2$ = 0.1067 |
| Extinction coefficient | 0.0077(5) |

Largest diff. peak and hole 0.293 and -0.395 e/Å$^3$

**Table 2.** Atomic coordinates (x $10^4$) and equivalent isotropic displacement parameters (Å$^2$ x $10^3$) for C40 H60 F12 N6 O8 S4.

$U_{eq}$ is defined as one third of the trace of the orthogonalized Uij tensor.

| | Occ. | x | y | z | $U_{eq}$ |
|---|---|---|---|---|---|
| N(1) | 1 | 7930(2) | 4496(1) | 5858(1) | 31(1) |
| C(2) | 1 | 7780(2) | 3466(2) | 6305(1) | 35(1) |
| N(3) | 1 | 9449(2) | 3551(1) | 6620(1) | 39(1) |
| C(4) | 1 | 10701(3) | 4659(2) | 6367(1) | 44(1) |
| C(5) | 1 | 9764(3) | 5257(2) | 5892(1) | 40(1) |
| C(6) | 1 | 6434(2) | 4752(2) | 5418(1) | 28(1) |
| C(7) | 1 | 5759(2) | 3478(2) | 5253(1) | 31(1) |
| C(8) | 1 | 5697(2) | 6276(2) | 5171(1) | 30(1) |
| C(9) | 0.625(6) | 10116(13) | 2655(11) | 7133(3) | 42(1) |
| C(10) | 0.625(6) | 7966(10) | 2390(9) | 7462(3) | 43(2) |
| C(11) | 0.625(6) | 8508(9) | 1345(6) | 8000(2) | 48(1) |
| C(12) | 0.625(6) | 6310(10) | 1049(5) | 8323(2) | 55(1) |
| C(13) | 0.625(6) | 6666(10) | -190(5) | 8824(2) | 57(1) |
| C(14) | 0.625(6) | 4459(11) | -484(5) | 9120(2) | 64(1) |
| C(15) | 0.625(6) | 4716(11) | -1777(5) | 9601(2) | 63(1) |
| C(16) | 0.625(6) | 2500(11) | -2033(5) | 9898(2) | 68(1) |
| C(17) | 0.625(6) | 2707(11) | -3355(5) | 10373(2) | 62(1) |
| C(18) | 0.625(6) | 494(10) | -3621(6) | 10670(2) | 67(1) |
| C(19) | 0.625(6) | 745(10) | -4947(6) | 11145(2) | 68(1) |
| C(20) | 0.625(6) | -1483(11) | -5268(8) | 11437(2) | 86(2) |
| C(9') | 0.375(6) | 9499(19) | 2542(17) | 7197(4) | 37(2) |
| C(10') | 0.375(6) | 7226(17) | 2321(15) | 7485(4) | 38(2) |
| C(11') | 0.375(6) | 7552(13) | 1349(9) | 8043(3) | 38(2) |
| C(12') | 0.375(6) | 5286(13) | 931(9) | 8294(3) | 46(2) |
| C(13') | 0.375(6) | 5512(14) | -102(8) | 8841(3) | 50(2) |
| C(14') | 0.375(6) | 3343(14) | -692(8) | 9062(2) | 57(2) |
| C(15') | 0.375(6) | 3526(14) | -1654(8) | 9618(3) | 52(2) |
| C(16') | 0.375(6) | 1416(15) | -2315(9) | 9835(2) | 64(2) |
| C(17') | 0.375(6) | 1563(14) | -3226(9) | 10403(3) | 54(2) |
| C(18') | 0.375(6) | -472(15) | -3955(9) | 10622(3) | 62(2) |
| C(19') | 0.375(6) | -327(16) | -4832(11) | 11188(3) | 67(2) |
| C(20') | 0.375(6) | -2394(18) | -5560(13) | 11405(4) | 84(3) |
| S(21) | 1 | 4497(1) | 9635(1) | 6098(1) | 31(1) |
| S(22) | 1 | 4147(1) | 7489(1) | 7033(1) | 33(1) |
| F(21) | 1 | 7(1) | 9849(1) | 6250(1) | 49(1) |
| F(22) | 1 | 1100(2) | 11306(1) | 5546(1) | 51(1) |
| F(23) | 1 | 1417(2) | 8818(1) | 5550(1) | 48(1) |
| F(24) | 1 | 7420(2) | 8889(1) | 7253(1) | 50(1) |
| F(25) | 1 | 8502(2) | 6430(1) | 7224(1) | 62(1) |
| F(26) | 1 | 6402(2) | 7197(2) | 7893(1) | 62(1) |
| O(21) | 1 | 4373(2) | 10900(1) | 6402(1) | 38(1) |
| O(22) | 1 | 5971(2) | 9644(1) | 5622(1) | 38(1) |
| O(23) | 1 | 3890(2) | 5875(1) | 7124(1) | 46(1) |
| O(24) | 1 | 2458(2) | 8615(1) | 7258(1) | 44(1) |
| N(21) | 1 | 4854(2) | 7920(1) | 6417(1) | 36(1) |

| | | | | | |
|---|---|---|---|---|---|
| C(21) | 1 | 1580(2) | 9899(2) | 5847(1) | 35(1) |
| C(22) | 1 | 6793(2) | 7500(2) | 7369(1) | 36(1) |

**Table 3.** Hydrogen coordinates (x $10^4$) and isotropic displacement parameters (Å$^2$ x $10^3$) for C40 H60 F12 N6 O8 S4.

| | Occ. | x | y | z | $U_{eq}$ |
|---|---|---|---|---|---|
| H(2) | 1 | 6671 | 2790 | 6385 | 42 |
| H(4) | 1 | 11994 | 4951 | 6502 | 53 |
| H(5) | 1 | 10265 | 6047 | 5631 | 48 |
| H(7) | 1 | 6286 | 2445 | 5429 | 38 |
| H(8) | 1 | 6180 | 7136 | 5289 | 36 |
| H(9A) | 0.625(6) | 11025 | 3236 | 7318 | 50 |
| H(9B) | 0.625(6) | 11083 | 1637 | 7081 | 50 |
| H(10A) | 0.625(6) | 7008 | 1891 | 7259 | 52 |
| H(10B) | 0.625(6) | 7060 | 3414 | 7530 | 52 |
| H(11A) | 0.625(6) | 9450 | 331 | 7934 | 58 |
| H(11B) | 0.625(6) | 9423 | 1858 | 8209 | 58 |
| H(12A) | 0.625(6) | 5285 | 717 | 8087 | 66 |
| H(12B) | 0.625(6) | 5504 | 2049 | 8433 | 66 |
| H(13A) | 0.625(6) | 7510 | -1186 | 8716 | 68 |
| H(13B) | 0.625(6) | 7641 | 156 | 9067 | 68 |
| H(14A) | 0.625(6) | 3448 | -755 | 8867 | 77 |
| H(14B) | 0.625(6) | 3668 | 501 | 9244 | 77 |
| H(15A) | 0.625(6) | 5476 | -2769 | 9477 | 76 |
| H(15B) | 0.625(6) | 5748 | -1517 | 9852 | 76 |
| H(16A) | 0.625(6) | 1454 | -2259 | 9643 | 81 |
| H(16B) | 0.625(6) | 1765 | -1047 | 10029 | 81 |
| H(17A) | 0.625(6) | 3449 | -4340 | 10242 | 75 |
| H(17B) | 0.625(6) | 3747 | -3126 | 10629 | 75 |
| H(18A) | 0.625(6) | -548 | -3855 | 10416 | 81 |
| H(18B) | 0.625(6) | -253 | -2638 | 10802 | 81 |
| H(19A) | 0.625(6) | 1548 | -5920 | 11014 | 82 |
| H(19B) | 0.625(6) | 1744 | -4692 | 11404 | 82 |
| H(20A) | 0.625(6) | -2291 | -4320 | 11573 | 129 |
| H(20B) | 0.625(6) | -1147 | -6119 | 11737 | 129 |
| H(20C) | 0.625(6) | -2462 | -5576 | 11190 | 129 |
| H(9C) | 0.375(6) | 10405 | 1490 | 7165 | 45 |
| H(9D) | 0.375(6) | 10353 | 3033 | 7426 | 45 |
| H(10C) | 0.375(6) | 6370 | 1787 | 7270 | 45 |
| H(10D) | 0.375(6) | 6289 | 3360 | 7521 | 45 |
| H(11C) | 0.375(6) | 8676 | 375 | 8014 | 46 |
| H(11D) | 0.375(6) | 8190 | 1954 | 8277 | 46 |
| H(12C) | 0.375(6) | 4619 | 378 | 8048 | 55 |
| H(12D) | 0.375(6) | 4193 | 1911 | 8335 | 55 |
| H(13C) | 0.375(6) | 6756 | -1013 | 8811 | 60 |
| H(13D) | 0.375(6) | 5984 | 505 | 9099 | 60 |
| H(14C) | 0.375(6) | 2916 | -1343 | 8812 | 68 |
| H(14D) | 0.375(6) | 2080 | 218 | 9074 | 68 |
| H(15C) | 0.375(6) | 4842 | -2533 | 9609 | 63 |
| H(15D) | 0.375(6) | 3885 | -985 | 9870 | 63 |
| H(16C) | 0.375(6) | 1096 | -3020 | 9591 | 76 |
| H(16D) | 0.375(6) | 88 | -1441 | 9830 | 76 |
| H(17C) | 0.375(6) | 2938 | -4066 | 10409 | 65 |
| H(17D) | 0.375(6) | 1823 | -2504 | 10646 | 65 |

| | | | | |
|---|---|---|---|---|
| H(18C) | 0.375(6) -716 | -4692 | 10382 | 74 |
| H(18D) | 0.375(6)-1853 | -3119 | 10610 | 74 |
| H(19C) | 0.375(6) 1049 | -5673 | 11200 | 81 |
| H(19D) | 0.375(6) -80 | -4098 | 11428 | 81 |
| H(20D) | 0.375(6)-3808 | -4794 | 11330 | 126 |
| H(20E) | 0.375(6)-2299 | -5876 | 11793 | 126 |
| H(20F) | 0.375(6)-2421 | -6482 | 11234 | 126 |

**Table 4.** Anisotropic parameters ($Å^2$ x $10^3$) for C40 H60 F12 N6 O8 S4.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [ h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12} ]$$

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| N(1) | 30(1) | 30(1) | 34(1) | -6(1) | -3(1) | -7(1) |
| C(2) | 37(1) | 31(1) | 36(1) | -5(1) | -7(1) | -5(1) |
| N(3) | 44(1) | 35(1) | 39(1) | -11(1) | -12(1) | 1(1) |
| C(4) | 38(1) | 47(1) | 53(1) | -19(1) | -10(1) | -8(1) |
| C(5) | 36(1) | 43(1) | 47(1) | -11(1) | -3(1) | -15(1) |
| C(6) | 28(1) | 28(1) | 30(1) | -5(1) | 1(1) | -7(1) |
| C(7) | 37(1) | 23(1) | 35(1) | -3(1) | -2(1) | -7(1) |
| C(8) | 36(1) | 24(1) | 34(1) | -6(1) | -1(1) | -10(1) |
| C(9) | 43(3) | 42(2) | 39(2) | -7(2) | -9(2) | -2(2) |
| C(10) | 49(4) | 35(2) | 42(2) | 0(1) | -5(3) | 0(2) |
| C(11) | 63(3) | 41(2) | 38(2) | -5(1) | -10(2) | -2(2) |
| C(12) | 69(3) | 46(2) | 42(2) | 1(1) | 0(3) | 4(2) |
| C(13) | 84(3) | 44(2) | 39(2) | 1(1) | -8(2) | -9(2) |
| C(14) | 82(3) | 57(2) | 48(2) | 5(2) | -1(2) | -7(2) |
| C(15) | 88(3) | 51(2) | 47(2) | 3(1) | -1(2) | -10(2) |
| C(16) | 87(3) | 61(2) | 48(2) | 5(2) | -5(2) | -6(2) |
| C(17) | 82(3) | 50(2) | 49(2) | 3(1) | 1(2) | -6(2) |
| C(18) | 73(3) | 66(3) | 51(2) | 9(2) | 0(2) | 2(2) |
| C(19) | 71(3) | 63(2) | 59(2) | 12(2) | 2(2) | -4(3) |
| C(20) | 66(4) | 104(4) | 68(3) | 20(3) | 12(3) | 0(3) |
| C(9') | 38(6) | 39(3) | 33(3) | 2(2) | -13(4) | -5(4) |
| C(10') | 39(5) | 38(3) | 32(2) | -2(2) | 4(3) | -2(3) |
| C(11') | 45(4) | 36(2) | 33(3) | -4(2) | -3(3) | -7(3) |
| C(12') | 44(4) | 49(3) | 41(3) | -1(2) | 6(3) | -8(3) |
| C(13') | 51(4) | 52(3) | 47(3) | -2(2) | -2(3) | -12(3) |
| C(14') | 64(4) | 62(3) | 44(3) | 5(2) | 2(3) | -22(3) |
| C(15') | 50(3) | 58(3) | 47(3) | 3(2) | 6(3) | -18(3) |
| C(16') | 72(4) | 78(4) | 46(3) | 1(3) | 4(3) | -38(3) |
| C(17') | 45(3) | 61(3) | 52(3) | 4(2) | 9(3) | -14(3) |
| C(18') | 66(4) | 77(4) | 50(3) | -4(3) | 4(3) | -40(3) |
| C(19') | 51(4) | 83(5) | 64(4) | 7(3) | 7(4) | -21(4) |
| C(20') | 79(6) | 108(6) | 78(5) | -15(4) | 23(5) | -61(5) |
| S(21) | 27(1) | 27(1) | 40(1) | -7(1) | -6(1) | -5(1) |
| S(22) | 23(1) | 31(1) | 44(1) | -3(1) | -9(1) | -6(1) |
| F(21) | 27(1) | 69(1) | 50(1) | -8(1) | -2(1) | -7(1) |
| F(22) | 45(1) | 41(1) | 62(1) | 5(1) | -17(1) | 0(1) |
| F(23) | 40(1) | 49(1) | 61(1) | -20(1) | -14(1) | -9(1) |
| F(24) | 39(1) | 50(1) | 69(1) | -13(1) | -11(1) | -19(1) |
| F(25) | 31(1) | 62(1) | 94(1) | -33(1) | -18(1) | 11(1) |
| F(26) | 55(1) | 87(1) | 44(1) | -1(1) | -16(1) | -17(1) |
| O(21) | 39(1) | 30(1) | 49(1) | -12(1) | -7(1) | -7(1) |
| O(22) | 32(1) | 38(1) | 44(1) | -8(1) | -2(1) | -8(1) |
| O(23) | 45(1) | 35(1) | 61(1) | 4(1) | -20(1) | -16(1) |
| O(24) | 26(1) | 48(1) | 53(1) | -4(1) | 0(1) | 0(1) |
| N(21) | 39(1) | 27(1) | 43(1) | -8(1) | -9(1) | -2(1) |
| C(21) | 31(1) | 33(1) | 42(1) | -6(1) | -7(1) | -4(1) |
| C(22) | 27(1) | 39(1) | 45(1) | -10(1) | -7(1) | -5(1) |

**Table 5.** Bond lengths [Å] and angles [°] for C40 H60 F12 N6 O8 S4

| | | | |
|---|---|---|---|
| N(1)-C(2) | 1.3397(18) | C(4)-N(3)-C(9') | 133.2(5) |
| N(1)-C(5) | 1.3841(18) | C(5)-C(4)-N(3) | 107.71(13) |
| N(1)-C(6) | 1.4366(17) | C(4)-C(5)-N(1) | 106.78(13) |
| C(2)-N(3) | 1.3307(18) | C(7)-C(6)-C(8) | 121.81(12) |
| N(3)-C(4) | 1.374(2) | C(7)-C(6)-N(1) | 119.28(12) |
| N(3)-C(9) | 1.449(7) | C(8)-C(6)-N(1) | 118.91(12) |
| N(3)-C(9') | 1.581(9) | C(6)-C(7)-C(8)#1 | 119.36(12) |
| C(4)-C(5) | 1.349(2) | C(6)-C(8)-C(7)#1 | 118.83(12) |
| C(6)-C(7) | 1.3844(19) | N(3)-C(9)-C(10) | 108.2(5) |
| C(6)-C(8) | 1.3893(18) | C(9)-C(10)-C(11) | 111.9(4) |
| C(7)-C(8)#1 | 1.3912(19) | C(12)-C(11)-C(10) | 111.3(4) |
| C(8)-C(7)#1 | 1.3912(19) | C(11)-C(12)-C(13) | 115.0(4) |
| C(9)-C(10) | 1.496(6) | C(14)-C(13)-C(12) | 113.4(4) |
| C(10)-C(11) | 1.536(6) | C(13)-C(14)-C(15) | 115.3(4) |
| C(11)-C(12) | 1.518(5) | C(16)-C(15)-C(14) | 114.6(4) |
| C(12)-C(13) | 1.532(5) | C(15)-C(16)-C(17) | 115.5(4) |
| C(13)-C(14) | 1.494(6) | C(18)-C(17)-C(16) | 115.7(4) |
| C(14)-C(15) | 1.521(5) | C(17)-C(18)-C(19) | 114.8(4) |
| C(15)-C(16) | 1.491(6) | C(20)-C(19)-C(18) | 115.4(4) |
| C(16)-C(17) | 1.527(5) | C(10')-C(9')-N(3) | 118.0(8) |
| C(17)-C(18) | 1.491(6) | C(9')-C(10')-C(11') | 111.9(7) |
| C(18)-C(19) | 1.529(6) | C(12')-C(11')-C(10') | 111.3(6) |
| C(19)-C(20) | 1.507(6) | C(11')-C(12')-C(13') | 113.9(5) |
| C(9')-C(10') | 1.505(9) | C(14')-C(13')-C(12') | 114.3(5) |
| C(10')-C(11') | 1.535(10) | C(13')-C(14')-C(15') | 114.5(6) |
| C(11')-C(12') | 1.515(7) | C(16')-C(15')-C(14') | 115.3(6) |
| C(12')-C(13') | 1.529(9) | C(15')-C(16')-C(17') | 115.3(6) |
| C(13')-C(14') | 1.500(8) | C(18')-C(17')-C(16') | 116.7(6) |
| C(14')-C(15') | 1.523(8) | C(17')-C(18')-C(19') | 116.3(6) |
| C(15')-C(16') | 1.496(7) | C(20')-C(19')-C(18') | 115.8(8) |
| C(16')-C(17') | 1.529(8) | O(22)-S(21)-O(21) | 117.90(6) |
| C(17')-C(18') | 1.490(7) | O(22)-S(21)-N(21) | 108.52(6) |
| C(18')-C(19') | 1.514(9) | O(21)-S(21)-N(21) | 117.15(6) |
| C(19')-C(20') | 1.504(8) | O(22)-S(21)-C(21) | 103.67(6) |
| S(21)-O(22) | 1.4300(10) | O(21)-S(21)-C(21) | 103.98(6) |
| S(21)-O(21) | 1.4374(10) | N(21)-S(21)-C(21) | 103.50(7) |
| S(21)-N(21) | 1.5746(12) | O(24)-S(22)-O(23) | 119.56(7) |
| S(21)-C(21) | 1.8402(14) | O(24)-S(22)-N(21) | 116.18(6) |
| S(22)-O(24) | 1.4229(11) | O(23)-S(22)-N(21) | 107.45(7) |
| S(22)-O(23) | 1.4309(11) | O(24)-S(22)-C(22) | 104.26(7) |
| S(22)-N(21) | 1.5880(13) | O(23)-S(22)-C(22) | 103.95(7) |
| S(22)-C(22) | 1.8338(14) | N(21)-S(22)-C(22) | 103.35(7) |
| F(21)-C(21) | 1.3258(17) | S(21)-N(21)-S(22) | 124.52(8) |
| F(22)-C(21) | 1.3367(17) | F(23)-C(21)-F(21) | 109.33(12) |
| F(23)-C(21) | 1.3217(17) | F(23)-C(21)-F(22) | 108.29(12) |
| F(24)-C(22) | 1.3188(17) | F(21)-C(21)-F(22) | 107.59(12) |
| F(25)-C(22) | 1.3189(17) | F(23)-C(21)-S(21) | 111.40(9) |
| F(26)-C(22) | 1.3231(18) | F(21)-C(21)-S(21) | 110.72(10) |
| | | F(22)-C(21)-S(21) | 109.40(10) |
| C(2)-N(1)-C(5) | 108.44(12) | F(25)-C(22)-F(24) | 108.94(12) |
| C(2)-N(1)-C(6) | 125.30(11) | F(25)-C(22)-F(26) | 108.55(13) |
| C(5)-N(1)-C(6) | 126.26(12) | F(24)-C(22)-F(26) | 108.45(12) |
| N(3)-C(2)-N(1) | 108.44(13) | F(25)-C(22)-S(22) | 111.28(10) |
| C(2)-N(3)-C(4) | 108.64(12) | F(24)-C(22)-S(22) | 110.36(10) |
| C(2)-N(3)-C(9) | 131.0(3) | F(26)-C(22)-S(22) | 109.19(10) |
| C(4)-N(3)-C(9) | 120.3(3) | | |
| C(2)-N(3)-C(9') | 117.9(5) | | |

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

**Table 6.** Torsion angles [°] for C40 H60 F12 N6 O8 S4.

| | | | |
|---|---|---|---|
| | | O(22)-S(21)-C(21)-F(22) | -64.19(11) |
| C(5)-N(1)-C(2)-N(3) | 0.02(16) | O(21)-S(21)-C(21)-F(22) | 59.65(11) |
| C(6)-N(1)-C(2)-N(3) | 179.82(12) | N(21)-S(21)-C(21)-F(22) | -177.43(10) |
| N(1)-C(2)-N(3)-C(4) | -0.16(16) | O(24)-S(22)-C(22)-F(25) | 176.11(11) |
| N(1)-C(2)-N(3)-C(9) | -176.9(5) | O(23)-S(22)-C(22)-F(25) | 50.12(13) |
| N(1)-C(2)-N(3)-C(9') | 175.0(6) | N(21)-S(22)-C(22)-F(25) | -62.00(12) |
| C(2)-N(3)-C(4)-C(5) | 0.24(17) | O(24)-S(22)-C(22)-F(24) | -62.81(11) |
| C(9)-N(3)-C(4)-C(5) | 177.4(4) | O(23)-S(22)-C(22)-F(24) | 171.19(10) |
| C(9')-N(3)-C(4)-C(5) | -173.8(7) | N(21)-S(22)-C(22)-F(24) | 59.08(11) |
| N(3)-C(4)-C(5)-N(1) | -0.22(17) | O(24)-S(22)-C(22)-F(26) | 56.31(12) |
| C(2)-N(1)-C(5)-C(4) | 0.13(16) | O(23)-S(22)-C(22)-F(26) | -69.69(12) |
| C(6)-N(1)-C(5)-C(4) | -179.67(13) | N(21)-S(22)-C(22)-F(26) | 178.20(10) |
| C(2)-N(1)-C(6)-C(7) | -40.40(19) | | |
| C(5)-N(1)-C(6)-C(7) | 139.36(14) | | |
| C(2)-N(1)-C(6)-C(8) | 139.39(13) | | |
| C(5)-N(1)-C(6)-C(8) | -40.85(19) | | |
| C(8)-C(6)-C(7)-C(8)#1 | 0.0(2) | | |
| N(1)-C(6)-C(7)-C(8)#1 | 179.74(11) | | |
| C(7)-C(6)-C(8)-C(7)#1 | 0.0(2) | | |
| N(1)-C(6)-C(8)-C(7)#1 | -179.74(11) | | |
| C(2)-N(3)-C(9)-C(10) | -39.6(9) | | |
| C(4)-N(3)-C(9)-C(10) | 144.0(5) | | |
| N(3)-C(9)-C(10)-C(11) | 175.9(6) | | |
| C(9)-C(10)-C(11)-C(12) | -178.4(6) | | |
| C(10)-C(11)-C(12)-C(13) | 170.6(5) | | |
| C(11)-C(12)-C(13)-C(14) | -178.2(4) | | |
| C(12)-C(13)-C(14)-C(15) | 176.4(4) | | |
| C(13)-C(14)-C(15)-C(16) | 178.9(4) | | |
| C(14)-C(15)-C(16)-C(17) | 178.4(4) | | |
| C(15)-C(16)-C(17)-C(18) | -179.7(4) | | |
| C(16)-C(17)-C(18)-C(19) | -179.9(4) | | |
| C(17)-C(18)-C(19)-C(20) | -177.9(5) | | |
| C(2)-N(3)-C(9')-C(10') | -34.7(13) | | |
| C(4)-N(3)-C(9')-C(10') | 138.9(8) | | |
| N(3)-C(9')-C(10')-C(11') | -178.7(10) | | |
| C(9')-C(10')-C(11')-C(12') | -171.5(9) | | |
| C(10')-C(11')-C(12')-C(13') | 177.4(8) | | |
| C(11')-C(12')-C(13')-C(14') | -172.6(6) | | |
| C(12')-C(13')-C(14')-C(15') | -177.1(6) | | |
| C(13')-C(14')-C(15')-C(16') | -177.3(7) | | |
| C(14')-C(15')-C(16')-C(17') | -177.6(6) | | |
| C(15')-C(16')-C(17')-C(18') | -177.6(7) | | |
| C(16')-C(17')-C(18')-C(19') | -179.0(7) | | |
| C(17')-C(18')-C(19')-C(20') | 179.8(8) | | |
| O(22)-S(21)-N(21)-S(22) | 161.23(8) | | |
| O(21)-S(21)-N(21)-S(22) | 24.64(12) | | |
| C(21)-S(21)-N(21)-S(22) | -89.09(10) | | |
| O(24)-S(22)-N(21)-S(21) | 21.01(12) | | |
| O(23)-S(22)-N(21)-S(21) | 157.97(9) | | |
| C(22)-S(22)-N(21)-S(21) | -92.49(10) | | |
| O(22)-S(21)-C(21)-F(23) | 55.50(11) | | |
| O(21)-S(21)-C(21)-F(23) | 179.34(10) | | |
| N(21)-S(21)-C(21)-F(23) | -57.74(11) | | |
| O(22)-S(21)-C(21)-F(21) | 177.40(10) | | |
| O(21)-S(21)-C(21)-F(21) | -58.76(11) | | |
| N(21)-S(21)-C(21)-F(21) | 64.16(11) | | |

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Symmetry transformations used to generate equivalent atoms:#1 -x+1,-y+1,-z+1

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