# Appendix 1

## Crystal data and structure refinement for **8**

Table 1.  Crystal data and structure refinement for Zntiof.

| | |
|---|---|
| Identification code | zntiof_abs |
| Empirical formula | $C_{44} H_{60} S_{12} Zn_2$ |
| Formula weight | 1104.54 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| Space group | C 2/c |
| Unit cell dimensions | a = 29.1118(19) Å          a= 90º |
| | b = 6.4571(4) Å          b= 112.5790(10)º. |
| | c = 28.8391(19) Å          g = 90º. |
| Volume | 5005.6(6) $Å^3$ |
| Z | 4 |
| Density (calculated) | 1.465 $Mg/m^3$ |
| Absorption coefficient | 1.490 $mm^{-1}$ |
| F(000) | 2304 |
| Crystal size | 0.34 x 0.14 x 0.05 $mm^3$ |
| Theta range for data collection | 2.53 to 26.50º. |
| Index ranges | -36<=h<=14, -7<=k<=7, -35<=l<=35 |
| Reflections collected | 12744 |
| Independent reflections | 4712 [R(int) = 0.0354] |
| Completeness to theta = 25.00º | 99.5 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.928 and 0.734 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 4712 / 0 / 382 |
| Goodness-of-fit on $F^2$ | 1.082 |
| Final R indices [I>2sigma(I)] | R1 = 0.0324, wR2 = 0.0718 |
| R indices (all data) | R1 = 0.0582, wR2 = 0.0838 |
| Extinction coefficient | 0 |
| Largest diff. peak and hole | 0.272 and -0.401 $e.Å^{-3}$ |

Table 2.  Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2$x $10^3$) for Zntiof.
U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Zn(1) | 491(1) | 2776(1) | 329(1) | 47(1) |
| S(1) | 1116(1) | 3935(1) | 1089(1) | 43(1) |
| S(2) | 794(1) | -360(1) | 836(1) | 48(1) |
| S(3) | 1786(1) | 2517(1) | 2214(1) | 43(1) |
| S(4) | -359(1) | 3361(1) | 209(1) | 41(1) |
| S(5) | 446(1) | 2323(1) | -498(1) | 44(1) |
| S(6) | 220(1) | 6496(1) | 1646(1) | 43(1) |
| C(1) | 1141(1) | 1401(4) | 1259(1) | 35(1) |
| C(2) | 1451(1) | 749(4) | 1761(1) | 35(1) |
| C(3) | 1528(1) | -1214(5) | 1957(1) | 42(1) |
| C(4) | 1847(1) | -1275(5) | 2459(1) | 42(1) |
| C(5) | 2022(1) | 612(4) | 2660(1) | 38(1) |
| C(6) | 2374(1) | 1098(5) | 3184(1) | 45(1) |
| C(7) | 2367(1) | 3315(5) | 3355(1) | 43(1) |
| C(8) | 2712(1) | 3652(5) | 3899(1) | 47(1) |
| C(9) | 2726(1) | 5858(5) | 4075(1) | 51(1) |
| C(10) | 3058(2) | 6189(6) | 4618(1) | 62(1) |
| C(11) | 3080(2) | 8401(8) | 4791(2) | 83(1) |
| C(12) | -270(1) | 5216(4) | 665(1) | 36(1) |
| C(13) | -37(1) | 4650(4) | 1185(1) | 36(1) |
| C(14) | 45(1) | 2690(5) | 1390(1) | 45(1) |
| C(15) | 310(1) | 2714(5) | 1907(1) | 49(1) |
| C(16) | 438(1) | 4649(5) | 2107(1) | 42(1) |
| C(17) | 743(2) | 5185(5) | 2642(1) | 55(1) |
| C(18) | 774(1) | 7455(5) | 2782(1) | 45(1) |
| C(19) | 1104(1) | 7831(5) | 3329(1) | 50(1) |
| C(20) | 1140(1) | 10073(5) | 3483(1) | 53(1) |
| C(21) | 1466(2) | 10440(6) | 4028(1) | 66(1) |
| C(22) | 1486(2) | 12655(8) | 4195(2) | 86(1) |

137

Table 3.   Bond lengths [Å] and angles [º] for Zntiof.
_____

| | | | |
|---|---|---|---|
| Zn(1)-S(5) | 2.3543(8) | C(10)-H(10B) | 0.95(4) |
| Zn(1)-S(1) | 2.3697(7) | C(11)-H(11A) | 0.93(5) |
| Zn(1)-S(4) | 2.3924(8) | C(11)-H(11B) | 0.97(4) |
| Zn(1)-S(2) | 2.4540(8) | C(11)-H(11C) | 0.96(4) |
| Zn(1)-S(4)#1 | 2.8840(8) | C(12)-C(13) | 1.435(4) |
| S(1)-C(1) | 1.701(3) | C(12)-S(5)#1 | 1.683(3) |
| S(2)-C(1) | 1.690(3) | C(13)-C(14) | 1.379(4) |
| S(3)-C(5) | 1.721(3) | C(14)-C(15) | 1.391(4) |
| S(3)-C(2) | 1.727(3) | C(14)-H(14) | 0.98(3) |
| S(4)-C(12) | 1.723(3) | C(15)-C(16) | 1.366(4) |
| S(5)-C(12)#1 | 1.683(3) | C(15)-H(15) | 0.88(3) |
| S(6)-C(16) | 1.715(3) | C(16)-C(17) | 1.497(4) |
| S(6)-C(13) | 1.729(3) | C(17)-C(18) | 1.513(4) |
| C(1)-C(2) | 1.444(3) | C(17)-H(17A) | 0.98(4) |
| C(2)-C(3) | 1.371(4) | C(17)-H(17B) | 0.98(4) |
| C(3)-C(4) | 1.388(4) | C(18)-C(19) | 1.519(4) |
| C(3)-H(3) | 0.89(3) | C(18)-H(18A) | 0.98(3) |
| C(4)-C(5) | 1.362(4) | C(18)-H(18B) | 0.98(3) |
| C(4)-H(4) | 0.90(3) | C(19)-C(20) | 1.507(5) |
| C(5)-C(6) | 1.498(4) | C(19)-H(19A) | 1.00(3) |
| C(6)-C(7) | 1.517(4) | C(19)-H(19B) | 0.94(4) |
| C(6)-H(6A) | 0.95(3) | C(20)-C(21) | 1.511(4) |
| C(6)-H(6B) | 0.94(3) | C(20)-H(20A) | 0.93(3) |
| C(7)-C(8) | 1.519(4) | C(20)-H(20B) | 0.99(4) |
| C(7)-H(7A) | 0.96(3) | C(21)-C(22) | 1.503(6) |
| C(7)-H(7B) | 1.00(3) | C(21)-H(21A) | 1.10(4) |
| C(8)-C(9) | 1.507(4) | C(21)-H(21B) | 0.92(5) |
| C(8)-H(8A) | 1.05(3) | C(22)-H(22A) | 0.91(5) |
| C(8)-H(8B) | 0.97(3) | C(22)-H(22B) | 0.98(5) |
| C(9)-C(10) | 1.505(4) | C(22)-H(22C) | 0.87(5) |
| C(9)-H(9A) | 1.02(3) | | |
| C(9)-H(9B) | 0.97(3) | S(5)-Zn(1)-S(1) | 134.47(3) |
| C(10)-C(11) | 1.507(6) | S(5)-Zn(1)-S(4) | 102.78(3) |
| C(10)-H(10A) | 0.99(4) | S(1)-Zn(1)-S(4) | 117.86(3) |

| | | | |
|---|---|---|---|
| S(5)-Zn(1)-S(2) | 111.59(3) | C(8)-C(7)-H(7A) | 110.1(17) |
| S(1)-Zn(1)-S(2) | 74.74(3) | C(6)-C(7)-H(7B) | 108.4(17) |
| S(4)-Zn(1)-S(2) | 109.35(3) | C(8)-C(7)-H(7B) | 111.9(17) |
| S(5)-Zn(1)-S(4)#1 | 67.62(2) | H(7A)-C(7)-H(7B) | 104(2) |
| S(1)-Zn(1)-S(4)#1 | 96.96(3) | C(9)-C(8)-C(7) | 113.9(3) |
| S(4)-Zn(1)-S(4)#1 | 82.43(3) | C(9)-C(8)-H(8A) | 109.9(17) |
| S(2)-Zn(1)-S(4)#1 | 167.72(3) | C(7)-C(8)-H(8A) | 107.5(17) |
| C(1)-S(1)-Zn(1) | 83.99(9) | C(9)-C(8)-H(8B) | 113.6(18) |
| C(1)-S(2)-Zn(1) | 81.59(9) | C(7)-C(8)-H(8B) | 105.6(19) |
| C(5)-S(3)-C(2) | 92.31(13) | H(8A)-C(8)-H(8B) | 106(2) |
| C(12)-S(4)-Zn(1) | 98.94(9) | C(10)-C(9)-C(8) | 114.1(3) |
| C(12)#1-S(5)-Zn(1) | 93.72(9) | C(10)-C(9)-H(9A) | 108.4(18) |
| C(16)-S(6)-C(13) | 92.21(13) | C(8)-C(9)-H(9A) | 110.5(18) |
| C(2)-C(1)-S(2) | 119.9(2) | C(10)-C(9)-H(9B) | 106.9(18) |
| C(2)-C(1)-S(1) | 120.67(19) | C(8)-C(9)-H(9B) | 112.8(18) |
| S(2)-C(1)-S(1) | 119.44(15) | H(9A)-C(9)-H(9B) | 104(2) |
| C(3)-C(2)-C(1) | 128.6(2) | C(9)-C(10)-C(11) | 114.2(4) |
| C(3)-C(2)-S(3) | 110.1(2) | C(9)-C(10)-H(10A) | 104(2) |
| C(1)-C(2)-S(3) | 121.3(2) | C(11)-C(10)-H(10A) | 117(2) |
| C(2)-C(3)-C(4) | 113.2(3) | C(9)-C(10)-H(10B) | 108(2) |
| C(2)-C(3)-H(3) | 122(2) | C(11)-C(10)-H(10B) | 110(2) |
| C(4)-C(3)-H(3) | 124(2) | H(10A)-C(10)-H(10B) | 104(3) |
| C(5)-C(4)-C(3) | 114.2(3) | C(10)-C(11)-H(11A) | 116(3) |
| C(5)-C(4)-H(4) | 124(2) | C(10)-C(11)-H(11B) | 107(3) |
| C(3)-C(4)-H(4) | 122(2) | H(11A)-C(11)-H(11B) | 107(4) |
| C(4)-C(5)-C(6) | 128.1(3) | C(10)-C(11)-H(11C) | 113(2) |
| C(4)-C(5)-S(3) | 110.2(2) | H(11A)-C(11)-H(11C) | 101(4) |
| C(6)-C(5)-S(3) | 121.8(2) | H(11B)-C(11)-H(11C) | 113(4) |
| C(5)-C(6)-C(7) | 115.9(2) | C(13)-C(12)-S(5)#1 | 120.6(2) |
| C(5)-C(6)-H(6A) | 106.7(17) | C(13)-C(12)-S(4) | 119.5(2) |
| C(7)-C(6)-H(6A) | 109.2(18) | S(5)#1-C(12)-S(4) | 119.84(15) |
| C(5)-C(6)-H(6B) | 107(2) | C(14)-C(13)-C(12) | 128.1(3) |
| C(7)-C(6)-H(6B) | 110(2) | C(14)-C(13)-S(6) | 110.4(2) |
| H(6A)-C(6)-H(6B) | 108(3) | C(12)-C(13)-S(6) | 121.3(2) |
| C(6)-C(7)-C(8) | 112.6(3) | C(13)-C(14)-C(15) | 112.6(3) |
| C(6)-C(7)-H(7A) | 109.5(18) | C(13)-C(14)-H(14) | 122.0(19) |

| | | | |
|---|---|---|---|
| C(15)-C(14)-H(14) | 125.3(19) | C(20)-C(19)-H(19B) | 112(2) |
| C(16)-C(15)-C(14) | 114.3(3) | C(18)-C(19)-H(19B) | 109(2) |
| C(16)-C(15)-H(15) | 124.6(19) | H(19A)-C(19)-H(19B) | 105(3) |
| C(14)-C(15)-H(15) | 121.1(19) | C(19)-C(20)-C(21) | 113.8(3) |
| C(15)-C(16)-C(17) | 127.1(3) | C(19)-C(20)-H(20A) | 107(2) |
| C(15)-C(16)-S(6) | 110.5(2) | C(21)-C(20)-H(20A) | 109(2) |
| C(17)-C(16)-S(6) | 122.3(2) | C(19)-C(20)-H(20B) | 111(2) |
| C(16)-C(17)-C(18) | 116.7(3) | C(21)-C(20)-H(20B) | 107(2) |
| C(16)-C(17)-H(17A) | 102(2) | H(20A)-C(20)-H(20B) | 109(3) |
| C(18)-C(17)-H(17A) | 108(2) | C(22)-C(21)-C(20) | 114.4(4) |
| C(16)-C(17)-H(17B) | 103(2) | C(22)-C(21)-H(21A) | 110(2) |
| C(18)-C(17)-H(17B) | 112(2) | C(20)-C(21)-H(21A) | 107(2) |
| H(17A)-C(17)-H(17B) | 116(3) | C(22)-C(21)-H(21B) | 112(3) |
| C(17)-C(18)-C(19) | 112.3(3) | C(20)-C(21)-H(21B) | 107(3) |
| C(17)-C(18)-H(18A) | 105.2(16) | H(21A)-C(21)-H(21B) | 106(4) |
| C(19)-C(18)-H(18A) | 111.5(16) | C(21)-C(22)-H(22A) | 105(3) |
| C(17)-C(18)-H(18B) | 109.1(17) | C(21)-C(22)-H(22B) | 111(3) |
| C(19)-C(18)-H(18B) | 108.5(17) | H(22A)-C(22)-H(22B) | 112(5) |
| H(18A)-C(18)-H(18B) | 110(2) | C(21)-C(22)-H(22C) | 110(3) |
| C(20)-C(19)-C(18) | 113.9(3) | H(22A)-C(22)-H(22C) | 107(4) |
| C(20)-C(19)-H(19A) | 108.8(17) | H(22B)-C(22)-H(22C) | 112(4) |
| C(18)-C(19)-H(19A) | 108.2(18) | | |

_____

Symmetry transformations used to generate equivalent atoms:

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

Table 4.   Anisotropic displacement parameters ($^2$x 10$^3$)for Zntiof.  The anisotropic displacement
factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

|        | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|--------|----------|----------|----------|----------|----------|----------|
| Zn(1)  | 45(1)    | 57(1)    | 28(1)    | -4(1)    | 3(1)     | 6(1)     |
| S(1)   | 48(1)    | 35(1)    | 34(1)    | -1(1)    | 1(1)     | -2(1)    |
| S(2)   | 55(1)    | 38(1)    | 34(1)    | -7(1)    | -1(1)    | -3(1)    |
| S(3)   | 51(1)    | 33(1)    | 31(1)    | -2(1)    | -1(1)    | -3(1)    |
| S(4)   | 44(1)    | 40(1)    | 31(1)    | -8(1)    | 6(1)     | -3(1)    |
| S(5)   | 55(1)    | 40(1)    | 32(1)    | -2(1)    | 11(1)    | 9(1)     |
| S(6)   | 54(1)    | 37(1)    | 29(1)    | -2(1)    | 7(1)     | 1(1)     |
| C(1)   | 35(1)    | 34(2)    | 32(1)    | -4(1)    | 9(1)     | 0(1)     |
| C(2)   | 34(1)    | 36(2)    | 29(1)    | -3(1)    | 5(1)     | 0(1)     |
| C(3)   | 43(2)    | 36(2)    | 37(2)    | -5(1)    | 5(1)     | -5(1)    |
| C(4)   | 51(2)    | 34(2)    | 36(2)    | 4(1)     | 9(1)     | 0(1)     |
| C(5)   | 41(1)    | 39(2)    | 27(1)    | 0(1)     | 5(1)     | 0(1)     |
| C(6)   | 48(2)    | 45(2)    | 31(2)    | -1(1)    | 2(1)     | 1(1)     |
| C(7)   | 44(2)    | 47(2)    | 32(2)    | -2(1)    | 6(1)     | 4(1)     |
| C(8)   | 51(2)    | 49(2)    | 32(2)    | -4(1)    | 6(1)     | -1(2)    |
| C(9)   | 55(2)    | 51(2)    | 38(2)    | -5(2)    | 8(2)     | 0(2)     |
| C(10)  | 74(2)    | 58(2)    | 43(2)    | -13(2)   | 9(2)     | 1(2)     |
| C(11)  | 99(4)    | 69(3)    | 68(3)    | -30(2)   | 19(3)    | -6(3)    |
| C(12)  | 35(1)    | 39(2)    | 32(1)    | -7(1)    | 10(1)    | -5(1)    |
| C(13)  | 38(1)    | 38(2)    | 30(1)    | -4(1)    | 10(1)    | -2(1)    |
| C(14)  | 56(2)    | 40(2)    | 36(2)    | -2(1)    | 14(1)    | -6(1)    |
| C(15)  | 65(2)    | 39(2)    | 38(2)    | 9(2)     | 16(2)    | 2(2)     |
| C(16)  | 47(2)    | 45(2)    | 29(2)    | 1(1)     | 9(1)     | 2(1)     |
| C(17)  | 66(2)    | 55(2)    | 33(2)    | -2(2)    | 8(2)     | 2(2)     |
| C(18)  | 45(2)    | 52(2)    | 33(2)    | -2(1)    | 10(1)    | 2(1)     |
| C(19)  | 57(2)    | 53(2)    | 32(2)    | -3(2)    | 7(2)     | -1(2)    |
| C(20)  | 56(2)    | 54(2)    | 43(2)    | -4(2)    | 12(2)    | 4(2)     |
| C(21)  | 86(3)    | 60(2)    | 40(2)    | -10(2)   | 13(2)    | -10(2)   |
| C(22)  | 100(4)   | 75(3)    | 73(3)    | -31(3)   | 24(3)    | -9(3)    |

Table 5.   Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($\text{Å}^2$x $10^3$) for Zntiof.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3) | 1387(11) | -2320(50) | 1775(12) | 50(9) |
| H(4) | 1922(11) | -2470(50) | 2632(11) | 53(9) |
| H(6A) | 2699(11) | 780(40) | 3200(10) | 52(9) |
| H(6B) | 2299(12) | 190(50) | 3400(12) | 67(11) |
| H(7A) | 2032(11) | 3700(40) | 3307(10) | 50(8) |
| H(7B) | 2450(10) | 4250(50) | 3123(11) | 55(9) |
| H(8A) | 3068(12) | 3180(50) | 3936(11) | 61(9) |
| H(8B) | 2606(11) | 2670(50) | 4091(12) | 55(10) |
| H(9A) | 2376(12) | 6360(50) | 4022(12) | 64(10) |
| H(9B) | 2833(11) | 6820(50) | 3880(12) | 52(9) |
| H(10A) | 3377(14) | 5540(60) | 4651(13) | 80(12) |
| H(10B) | 2939(12) | 5320(60) | 4816(13) | 74(12) |
| H(11A) | 3295(16) | 8650(70) | 5122(18) | 114(16) |
| H(11B) | 2747(16) | 8770(70) | 4764(16) | 105(16) |
| H(11C) | 3209(14) | 9320(60) | 4611(14) | 79(14) |
| H(14) | -90(11) | 1450(50) | 1187(12) | 69(10) |
| H(15) | 382(10) | 1560(50) | 2082(11) | 45(8) |
| H(17A) | 1078(14) | 4730(60) | 2680(13) | 86(12) |
| H(17B) | 584(13) | 4360(60) | 2827(14) | 89(13) |
| H(18A) | 429(10) | 7880(40) | 2708(10) | 42(8) |
| H(18B) | 910(10) | 8230(40) | 2571(11) | 49(9) |
| H(19A) | 1445(12) | 7310(40) | 3387(12) | 56(9) |
| H(19B) | 994(13) | 7000(50) | 3532(14) | 75(12) |
| H(20A) | 819(13) | 10520(50) | 3424(12) | 65(10) |
| H(20B) | 1277(12) | 10930(60) | 3279(13) | 77(12) |
| H(21A) | 1841(16) | 9910(60) | 4082(14) | 104(14) |
| H(21B) | 1355(17) | 9560(70) | 4217(17) | 120(18) |
| H(22A) | 1610(18) | 13370(80) | 3998(18) | 120(20) |
| H(22B) | 1160(20) | 13150(80) | 4160(20) | 150(20) |
| H(22C) | 1698(18) | 12780(70) | 4502(19) | 111(18) |

Table 6.  Torsion angles [º] for Zntiof.

_____

| | | | |
|---|---|---|---|
| S(5)-Zn(1)-S(1)-C(1) | -108.43(10) | C(3)-C(4)-C(5)-S(3) | -0.3(3) |
| S(4)-Zn(1)-S(1)-C(1) | 101.16(9) | C(2)-S(3)-C(5)-C(4) | 0.4(2) |
| S(2)-Zn(1)-S(1)-C(1) | -2.98(9) | C(2)-S(3)-C(5)-C(6) | 179.3(3) |
| S(4)#1-Zn(1)-S(1)-C(1) | -173.75(9) | C(4)-C(5)-C(6)-C(7) | -159.7(3) |
| S(5)-Zn(1)-S(2)-C(1) | 135.31(9) | S(3)-C(5)-C(6)-C(7) | 21.5(4) |
| S(1)-Zn(1)-S(2)-C(1) | 3.01(9) | C(5)-C(6)-C(7)-C(8) | 176.6(3) |
| S(4)-Zn(1)-S(2)-C(1) | -111.67(9) | C(6)-C(7)-C(8)-C(9) | 178.0(3) |
| S(4)#1-Zn(1)-S(2)-C(1) | 51.47(16) | C(7)-C(8)-C(9)-C(10) | 178.5(3) |
| S(5)-Zn(1)-S(4)-C(12) | -141.90(10) | C(8)-C(9)-C(10)-C(11) | 179.0(4) |
| S(1)-Zn(1)-S(4)-C(12) | 16.91(10) | Zn(1)-S(4)-C(12)-C(13) | -68.6(2) |
| S(2)-Zn(1)-S(4)-C(12) | 99.44(10) | Zn(1)-S(4)-C(12)-S(5)#1 | 110.40(14) |
| S(4)#1-Zn(1)-S(4)-C(12) | -76.99(10) | S(5)#1-C(12)-C(13)-C(14) | 166.7(2) |
| S(1)-Zn(1)-S(5)-C(12)#1 | -87.05(9) | S(4)-C(12)-C(13)-C(14) | -14.3(4) |
| S(4)-Zn(1)-S(5)-C(12)#1 | 66.35(9) | S(5)#1-C(12)-C(13)-S(6) | -17.6(3) |
| S(2)-Zn(1)-S(5)-C(12)#1 | -176.57(9) | S(4)-C(12)-C(13)-S(6) | 161.40(15) |
| S(4)#1-Zn(1)-S(5)-C(12)#1 | -9.80(9) | C(16)-S(6)-C(13)-C(14) | 0.4(2) |
| Zn(1)-S(2)-C(1)-C(2) | 174.7(2) | C(16)-S(6)-C(13)-C(12) | -176.0(2) |
| Zn(1)-S(2)-C(1)-S(1) | -4.65(14) | C(12)-C(13)-C(14)-C(15) | 175.9(3) |
| Zn(1)-S(1)-C(1)-C(2) | -174.5(2) | S(6)-C(13)-C(14)-C(15) | -0.1(3) |
| Zn(1)-S(1)-C(1)-S(2) | 4.79(15) | C(13)-C(14)-C(15)-C(16) | -0.3(4) |
| S(2)-C(1)-C(2)-C(3) | 2.9(4) | C(14)-C(15)-C(16)-C(17) | -176.9(3) |
| S(1)-C(1)-C(2)-C(3) | -177.8(2) | C(14)-C(15)-C(16)-S(6) | 0.6(4) |
| S(2)-C(1)-C(2)-S(3) | -176.61(15) | C(13)-S(6)-C(16)-C(15) | -0.6(2) |
| S(1)-C(1)-C(2)-S(3) | 2.7(3) | C(13)-S(6)-C(16)-C(17) | 177.0(3) |
| C(5)-S(3)-C(2)-C(3) | -0.3(2) | C(15)-C(16)-C(17)-C(18) | -172.1(3) |
| C(5)-S(3)-C(2)-C(1) | 179.2(2) | S(6)-C(16)-C(17)-C(18) | 10.7(5) |
| C(1)-C(2)-C(3)-C(4) | -179.3(3) | C(16)-C(17)-C(18)-C(19) | -178.3(3) |
| S(3)-C(2)-C(3)-C(4) | 0.2(3) | C(17)-C(18)-C(19)-C(20) | -179.3(3) |
| C(2)-C(3)-C(4)-C(5) | 0.0(4) | C(18)-C(19)-C(20)-C(21) | 179.7(3) |
| C(3)-C(4)-C(5)-C(6) | -179.2(3) | C(19)-C(20)-C(21)-C(22) | -177.1(4) |

_____

Symmetry transformations used to generate equivalent atoms:

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

# Appendix 2

## Crystal data and structure refinement for **12**

Table 1.  Crystal data and structure refinement for MTSLReBT.

| | |
|---|---|
| Identification code | mtslrebm |
| Empirical formula | C13 H5 O4 Re S4 |
| Formula weight | 539.61 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | monoclinic |
| Space group | P2$_1$/n |
| Unit cell dimensions | a = 5.9892(4) Å   $\alpha$= 90°. |
| | b = 7.4933(5) Å   $\beta$= 93.8530(10)°. |
| | c = 35.247(3) Å   $\gamma$ = 90°. |
| Volume | 1578.27(19) Å$^3$ |
| Z | 4 |
| Density (calculated) | 2.271 Mg/m$^3$ |
| Absorption coefficient | 8.240 mm$^{-1}$ |
| F(000) | 1016 |
| Crystal size | 0.34 x 0.10 x 0.06 mm$^3$ |
| Theta range for data collection | 2.78 to 26.52°. |
| Index ranges | -7<=h<=3, -8<=k<=7, -42<=l<=43 |
| Reflections collected | 8226 |
| Independent reflections | 2996 [R(int) = 0.0305] |
| Completeness to theta = 25.00° | 99.6 % |
| Refinement method | Full-matrix least-squares on F$^2$ |
| Data / restraints / parameters | 2996 / 0 / 199 |
| Goodness-of-fit on F$^2$ | 1.242 |
| Final R indices [I>2sigma(I)] | R1 = 0.0286, wR2 = 0.0726 |
| R indices (all data) | R1 = 0.0318, wR2 = 0.0745 |
| Largest diff. peak and hole | 0.489 and -1.296 e.Å$^{-3}$ |

Table 2.  Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2$x $10^3$) for MTSLReBT. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Re(1) | 7478(1) | 2762(1) | 647(1) | 42(1) |
| S(1) | 10667(2) | 4037(2) | 1061(1) | 48(1) |
| S(2) | 6573(2) | 2737(2) | 1329(1) | 47(1) |
| S(3) | 8383(2) | 3220(2) | 2197(1) | 44(1) |
| S(4) | 12189(2) | 4199(2) | 3276(1) | 56(1) |
| C(1) | 4805(9) | 1596(9) | 425(2) | 57(1) |
| O(1) | 3271(7) | 882(7) | 297(1) | 80(1) |
| C(2) | 8732(10) | 2934(8) | 154(2) | 54(1) |
| O(2) | 9482(9) | 3069(7) | -129(1) | 78(1) |
| C(3) | 8889(9) | 380(8) | 740(2) | 52(1) |
| O(3) | 9672(8) | -977(7) | 802(1) | 75(1) |
| C(4) | 6109(9) | 5177(9) | 570(2) | 54(1) |
| O(4) | 5397(8) | 6543(7) | 518(1) | 80(1) |
| C(5) | 9162(7) | 3564(6) | 1441(1) | 37(1) |
| C(6) | 9994(7) | 3829(6) | 1828(1) | 37(1) |
| C(7) | 12010(8) | 4512(7) | 1964(1) | 43(1) |
| C(8) | 12250(8) | 4578(7) | 2364(2) | 46(1) |
| C(9) | 10420(7) | 3927(6) | 2535(1) | 39(1) |
| C(10) | 10113(8) | 3683(6) | 2932(1) | 40(1) |
| C(11) | 8261(9) | 2927(6) | 3093(2) | 44(1) |
| C(12) | 8636(10) | 2784(7) | 3496(2) | 51(1) |
| C(13) | 10655(10) | 3410(9) | 3626(2) | 57(1) |

145

Table 3.   Bond lengths [Å] and angles [°] for MTSLReBT.

| | | | |
|---|---|---|---|
| Re(1)-C(1) | 1.942(6) | C(3)-Re(1)-S(2) | 87.29(15) |
| Re(1)-C(2) | 1.943(6) | C(4)-Re(1)-S(2) | 91.33(15) |
| Re(1)-C(3) | 1.993(6) | C(1)-Re(1)-S(1) | 168.26(18) |
| Re(1)-C(4) | 1.998(6) | C(2)-Re(1)-S(1) | 99.75(18) |
| Re(1)-S(2) | 2.4974(14) | C(3)-Re(1)-S(1) | 87.01(16) |
| Re(1)-S(1) | 2.5124(12) | C(4)-Re(1)-S(1) | 91.33(16) |
| S(1)-C(5) | 1.701(4) | S(2)-Re(1)-S(1) | 69.54(4) |
| S(2)-C(5) | 1.692(5) | C(5)-S(1)-Re(1) | 87.42(16) |
| S(3)-C(9) | 1.729(5) | C(5)-S(2)-Re(1) | 88.12(16) |
| S(3)-C(6) | 1.733(4) | C(9)-S(3)-C(6) | 91.9(2) |
| S(4)-C(13) | 1.693(6) | C(13)-S(4)-C(10) | 91.9(3) |
| S(4)-C(10) | 1.721(5) | O(1)-C(1)-Re(1) | 178.5(6) |
| C(1)-O(1) | 1.131(7) | O(2)-C(2)-Re(1) | 178.4(6) |
| C(2)-O(2) | 1.128(7) | O(3)-C(3)-Re(1) | 178.2(5) |
| C(3)-O(3) | 1.134(7) | O(4)-C(4)-Re(1) | 177.4(6) |
| C(4)-O(4) | 1.120(7) | C(6)-C(5)-S(2) | 121.8(3) |
| C(5)-C(6) | 1.435(6) | C(6)-C(5)-S(1) | 123.4(3) |
| C(6)-C(7) | 1.368(6) | S(2)-C(5)-S(1) | 114.7(3) |
| C(7)-C(8) | 1.409(7) | C(7)-C(6)-C(5) | 128.9(4) |
| C(8)-C(9) | 1.374(6) | C(7)-C(6)-S(3) | 110.9(3) |
| C(9)-C(10) | 1.437(7) | C(5)-C(6)-S(3) | 120.2(3) |
| C(10)-C(11) | 1.398(7) | C(6)-C(7)-C(8) | 113.1(4) |
| C(11)-C(12) | 1.429(8) | C(9)-C(8)-C(7) | 113.2(4) |
| C(12)-C(13) | 1.348(8) | C(8)-C(9)-C(10) | 129.0(4) |
| | | C(8)-C(9)-S(3) | 110.7(4) |
| C(1)-Re(1)-C(2) | 91.5(2) | C(10)-C(9)-S(3) | 120.1(4) |
| C(1)-Re(1)-C(3) | 89.6(2) | C(11)-C(10)-C(9) | 127.1(4) |
| C(2)-Re(1)-C(3) | 91.2(2) | C(11)-C(10)-S(4) | 111.2(4) |
| C(1)-Re(1)-C(4) | 91.9(2) | C(9)-C(10)-S(4) | 121.6(4) |
| C(2)-Re(1)-C(4) | 89.9(2) | C(10)-C(11)-C(12) | 110.9(5) |
| C(3)-Re(1)-C(4) | 178.1(2) | C(13)-C(12)-C(11) | 112.9(5) |
| C(1)-Re(1)-S(2) | 99.09(17) | C(12)-C(13)-S(4) | 113.1(4) |
| C(2)-Re(1)-S(2) | 169.24(18) | | |

Symmetry transformations used to generate equivalent atoms:

Table 4.   Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$)for MTSLReBT.  The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2 a^{*2} U^{11} + ... + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Re(1) | 37(1) | 52(1) | 37(1) | -3(1) | 4(1) | -1(1) |
| S(1) | 38(1) | 68(1) | 39(1) | 0(1) | 7(1) | -10(1) |
| S(2) | 38(1) | 61(1) | 40(1) | -4(1) | 7(1) | -9(1) |
| S(3) | 37(1) | 57(1) | 39(1) | 3(1) | 4(1) | -6(1) |
| S(4) | 53(1) | 71(1) | 45(1) | -3(1) | 0(1) | -8(1) |
| C(1) | 48(3) | 68(4) | 55(3) | -8(3) | 11(3) | 4(3) |
| O(1) | 50(2) | 103(4) | 85(3) | -27(3) | -1(2) | -18(2) |
| C(2) | 51(3) | 58(4) | 52(4) | -1(3) | 9(3) | -5(2) |
| O(2) | 93(4) | 95(4) | 47(3) | -7(2) | 26(2) | -12(3) |
| C(3) | 50(3) | 64(4) | 43(3) | -5(3) | 14(2) | -6(3) |
| O(3) | 86(3) | 67(3) | 73(3) | 8(2) | 19(2) | 21(2) |
| C(4) | 53(3) | 72(4) | 35(3) | -4(3) | -4(2) | 2(3) |
| O(4) | 95(3) | 69(3) | 73(3) | 3(3) | -3(3) | 26(3) |
| C(5) | 38(2) | 37(2) | 38(2) | 0(2) | 9(2) | 2(2) |
| C(6) | 39(2) | 39(3) | 35(2) | 1(2) | 9(2) | 3(2) |
| C(7) | 41(2) | 44(3) | 45(3) | -3(2) | 8(2) | -7(2) |
| C(8) | 44(3) | 46(3) | 49(3) | -4(2) | 3(2) | -8(2) |
| C(9) | 41(2) | 35(2) | 40(3) | -2(2) | 1(2) | 2(2) |
| C(10) | 43(2) | 35(3) | 42(3) | -3(2) | -1(2) | 4(2) |
| C(11) | 55(3) | 40(3) | 36(3) | -1(2) | 7(2) | -3(2) |
| C(12) | 57(3) | 50(3) | 49(3) | 0(2) | 16(3) | 2(2) |
| C(13) | 71(4) | 64(4) | 36(3) | 0(3) | 3(3) | 0(3) |

Table 5.  Torsion angles [°] for MTSLReBT.

| | | | |
|---|---|---|---|
| C(1)-Re(1)-S(1)-C(5) | -12.4(9) | S(1)-Re(1)-C(4)-O(4) | 79(12) |
| C(2)-Re(1)-S(1)-C(5) | -176.3(2) | Re(1)-S(2)-C(5)-C(6) | -175.8(4) |
| C(3)-Re(1)-S(1)-C(5) | -85.6(2) | Re(1)-S(2)-C(5)-S(1) | 4.0(3) |
| C(4)-Re(1)-S(1)-C(5) | 93.6(2) | Re(1)-S(1)-C(5)-C(6) | 175.8(4) |
| S(2)-Re(1)-S(1)-C(5) | 2.63(16) | Re(1)-S(1)-C(5)-S(2) | -4.0(3) |
| C(1)-Re(1)-S(2)-C(5) | 174.3(3) | S(2)-C(5)-C(6)-C(7) | -178.5(4) |
| C(2)-Re(1)-S(2)-C(5) | 3.0(10) | S(1)-C(5)-C(6)-C(7) | 1.7(8) |
| C(3)-Re(1)-S(2)-C(5) | 85.2(2) | S(2)-C(5)-C(6)-S(3) | 2.5(6) |
| C(4)-Re(1)-S(2)-C(5) | -93.6(2) | S(1)-C(5)-C(6)-S(3) | -177.3(3) |
| S(1)-Re(1)-S(2)-C(5) | -2.65(17) | C(9)-S(3)-C(6)-C(7) | 1.0(4) |
| C(2)-Re(1)-C(1)-O(1) | 87(21) | C(9)-S(3)-C(6)-C(5) | -179.9(4) |
| C(3)-Re(1)-C(1)-O(1) | -4(21) | C(5)-C(6)-C(7)-C(8) | 179.9(5) |
| C(4)-Re(1)-C(1)-O(1) | 177(100) | S(3)-C(6)-C(7)-C(8) | -1.1(6) |
| S(2)-Re(1)-C(1)-O(1) | -91(21) | C(6)-C(7)-C(8)-C(9) | 0.6(7) |
| S(1)-Re(1)-C(1)-O(1) | -77(21) | C(7)-C(8)-C(9)-C(10) | 175.9(5) |
| C(1)-Re(1)-C(2)-O(2) | 147(22) | C(7)-C(8)-C(9)-S(3) | 0.2(6) |
| C(3)-Re(1)-C(2)-O(2) | -124(22) | C(6)-S(3)-C(9)-C(8) | -0.7(4) |
| C(4)-Re(1)-C(2)-O(2) | 55(22) | C(6)-S(3)-C(9)-C(10) | -176.8(4) |
| S(2)-Re(1)-C(2)-O(2) | -42(23) | C(8)-C(9)-C(10)-C(11) | -176.3(5) |
| S(1)-Re(1)-C(2)-O(2) | -36(22) | S(3)-C(9)-C(10)-C(11) | -1.0(7) |
| C(1)-Re(1)-C(3)-O(3) | -92(18) | C(8)-C(9)-C(10)-S(4) | -0.7(7) |
| C(2)-Re(1)-C(3)-O(3) | 176(100) | S(3)-C(9)-C(10)-S(4) | 174.6(3) |
| C(4)-Re(1)-C(3)-O(3) | 49(21) | C(13)-S(4)-C(10)-C(11) | 0.6(4) |
| S(2)-Re(1)-C(3)-O(3) | 7(18) | C(13)-S(4)-C(10)-C(9) | -175.7(4) |
| S(1)-Re(1)-C(3)-O(3) | 76(18) | C(9)-C(10)-C(11)-C(12) | 175.4(5) |
| C(1)-Re(1)-C(4)-O(4) | -112(12) | S(4)-C(10)-C(11)-C(12) | -0.6(5) |
| C(2)-Re(1)-C(4)-O(4) | -20(12) | C(10)-C(11)-C(12)-C(13) | 0.3(7) |
| C(3)-Re(1)-C(4)-O(4) | 107(13) | C(11)-C(12)-C(13)-S(4) | 0.2(7) |
| S(2)-Re(1)-C(4)-O(4) | 149(12) | C(10)-S(4)-C(13)-C(12) | -0.5(5) |

Symmetry transformations used to generate equivalent atoms: