# Appendix 1

## Crystallographic data of Complex 2

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

| | | |
|---|---|---|
| Identification code | db15 | |
| Empirical formula | $C_{16}$ $H_8$ $Mn_2$ $O_{10}$ S | |
| Formula weight | 502.16 | |
| Temperature | 293(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P $2_1$/c | |
| Unit cell dimensions | a = 7.920(4) Å | α= 90°. |
| | b = 22.236(11) Å | β= 95.591(7)°. |
| | c = 11.548(5) Å | γ = 90°. |
| Volume | 2024.0(16) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.648 $Mg/m^3$ | |
| Absorption coefficient | 1.400 $mm^{-1}$ | |
| F(000) | 1000 | |
| Crystal size | 0.40 x 0.30 x 0.18 $mm^3$ | |
| Theta range for data collection | 2.55 to 26.30°. | |
| Index ranges | -5<=h<=9, -24<=k<=27, -10<=l<=13 | |
| Reflections collected | 6741 | |
| Independent reflections | 3324 [R(int) = 0.0390] | |
| Completeness to theta = 25.00° | 89.3 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.777 and 0.476 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3324 / 0 / 271 | |
| Goodness-of-fit on $F^2$ | 1.106 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0582, wR2 = 0.1338 | |
| R indices (all data) | R1 = 0.0792, wR2 = 0.1431 | |
| Extinction coefficient | 0 | |
| Largest diff. peak and hole | 0.425 and -0.365 e.$Å^{-3}$ | |

**Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$)**

U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Mn(1) | 3948(1) | 6623(1) | 4314(1) | 56(1) |
| Mn(2) | 1394(1) | 6114(1) | 2591(1) | 44(1) |
| O(1) | 6582(7) | 7097(3) | 6054(5) | 131(3) |
| O(2) | 1042(7) | 7057(2) | 5549(4) | 78(1) |
| O(3) | 3657(7) | 7748(3) | 2928(5) | 96(2) |
| O(4) | 6457(6) | 6170(3) | 2763(5) | 108(2) |
| O(5) | 3736(8) | 5421(3) | 5463(5) | 102(2) |
| O(6) | -455(7) | 7265(2) | 2817(4) | 89(2) |
| O(7) | 3379(6) | 6684(2) | 826(4) | 79(1) |
| O(8) | 3674(7) | 5048(2) | 2541(5) | 96(2) |
| O(9) | -364(6) | 5699(2) | 4616(4) | 77(1) |
| C(1) | 5552(9) | 6907(4) | 5384(7) | 87(2) |
| C(2) | 2144(8) | 6883(3) | 5072(5) | 58(2) |
| C(3) | 3767(9) | 7313(3) | 3430(6) | 68(2) |
| C(4) | 5466(9) | 6340(4) | 3353(6) | 75(2) |
| C(5) | 3824(9) | 5876(4) | 5023(6) | 72(2) |
| C(6) | 239(8) | 6820(3) | 2707(5) | 55(2) |
| C(7) | 2599(7) | 6454(3) | 1490(6) | 54(2) |
| C(8) | 2782(8) | 5453(3) | 2583(5) | 61(2) |
| C(9) | 338(7) | 5847(3) | 3846(5) | 50(1) |
| C(10) | -307(12) | 5734(5) | 1518(8) | 45(3) |
| O(10) | -1172(7) | 5938(2) | 573(5) | 58(1) |
| C(11) | -968(17) | 5122(6) | 1641(10) | 53(4) |
| S(1) | -2679(3) | 4876(1) | 741(2) | 82(1) |
| C(12) | -474(19) | 4673(6) | 2432(9) | 73(4) |
| C(13) | -1450(30) | 4158(6) | 2251(14) | 102(6) |
| C(14) | -2691(14) | 4208(4) | 1418(9) | 99(3) |
| C(15) | -1030(14) | 6544(4) | 107(10) | 69(3) |
| C(16) | -2453(11) | 6607(5) | -825(10) | 97(4) |
| C(10A) | -240(90) | 5660(30) | 1540(60) | 52(19) |

| | | | | |
|---|---|---|---|---|
| O(10A) | -980(70) | 5130(30) | 1630(40) | 52(19) |
| C(11A) | -1130(70) | 5960(20) | 530(50) | 81(6) |
| S(1A) | -2810(20) | 5591(7) | -283(15) | 81(6) |
| C(12A) | -870(100) | 6520(20) | 50(70) | 81(6) |
| C(13A) | -1990(80) | 6649(17) | -940(60) | 81(6) |
| C(14A) | -3110(40) | 6183(13) | -1220(30) | 81(6) |
| C(15A) | -440(100) | 4700(40) | 2550(60) | 52(19) |
| C(16A) | -1560(100) | 4160(30) | 2360(70) | 52(19) |

**Table 3. Bond lengths [Å] and angles [°]**

| | | | |
|---|---|---|---|
| Mn(1)-C(1) | 1.798(7) | C(15)-C(16) | 1.487(9) |
| Mn(1)-C(4) | 1.825(8) | C(15)-H(15A) | 0.97 |
| Mn(1)-C(2) | 1.840(7) | C(15)-H(15B) | 0.97 |
| Mn(1)-C(3) | 1.841(8) | C(16)-H(16A) | 0.96 |
| Mn(1)-C(5) | 1.858(9) | C(16)-H(16B) | 0.96 |
| Mn(1)-Mn(2) | 2.9238(14) | C(16)-H(16C) | 0.96 |
| Mn(2)-C(7) | 1.826(7) | C(11)-C(12) | 1.384(10) |
| Mn(2)-C(6) | 1.828(7) | C(11)-S(1) | 1.715(10) |
| Mn(2)-C(8) | 1.836(7) | S(1)-C(14) | 1.679(10) |
| Mn(2)-C(9) | 1.841(6) | C(12)-C(13) | 1.386(12) |
| Mn(2)-C(10) | 1.933(7) | C(12)-H(12) | 0.93 |
| Mn(2)-C(10A) | 1.96(4) | C(13)-C(14) | 1.313(19) |
| O(1)-C(1) | 1.148(8) | C(13)-H(13) | 0.93 |
| O(2)-C(2) | 1.144(7) | C(14)-H(14) | 0.93 |
| O(3)-C(3) | 1.128(8) | C(10A)-O(10A) | 1.332 |
| O(4)-C(4) | 1.153(8) | C(10A)-C(11A) | 1.457 |
| O(5)-C(5) | 1.136(9) | O(10A)-C(15A) | 1.450 |
| O(6)-C(6) | 1.145(7) | C(15A)-C(16A) | 1.508 |
| O(7)-C(7) | 1.152(7) | C(15A)-H(15C) | 0.97 |
| O(8)-C(8) | 1.147(7) | C(15A)-H(15D) | 0.97 |
| O(9)-C(9) | 1.141(7) | C(16A)-H(16D) | 0.96 |
| C(10)-O(10) | 1.312(7) | C(16A)-H(16E) | 0.96 |
| C(10)-C(11) | 1.470(11) | C(16A)-H(16F) | 0.96 |
| O(10)-C(15) | 1.457(8) | C(11A)-C(12A) | 1.39 |

| | | | |
|---|---|---|---|
| C(11A)-S(1A) | 1.755 | C(9)-Mn(2)-C(10A) | 90(3) |
| S(1A)-C(14A) | 1.704 | C(10)-Mn(2)-C(10A) | 5(2) |
| C(12A)-C(13A) | 1.409 | C(7)-Mn(2)-Mn(1) | 86.54(18) |
| C(12A)-H(12A) | 0.93 | C(6)-Mn(2)-Mn(1) | 86.33(18) |
| C(13A)-C(14A) | 1.378 | C(8)-Mn(2)-Mn(1) | 86.45(19) |
| C(13A)-H(13A) | 0.93 | C(9)-Mn(2)-Mn(1) | 85.76(18) |
| C(14A)-H(14A) | 0.93 | C(10)-Mn(2)-Mn(1) | 176.3(3) |
| | | C(10A)-Mn(2)-Mn(1) | 171.9(17) |
| C(1)-Mn(1)-C(4) | 94.4(3) | O(1)-C(1)-Mn(1) | 178.8(9) |
| C(1)-Mn(1)-C(2) | 95.3(3) | O(2)-C(2)-Mn(1) | 178.4(6) |
| C(4)-Mn(1)-C(2) | 170.2(3) | O(3)-C(3)-Mn(1) | 177.3(7) |
| C(1)-Mn(1)-C(3) | 95.7(3) | O(4)-C(4)-Mn(1) | 178.3(6) |
| C(4)-Mn(1)-C(3) | 88.3(4) | O(5)-C(5)-Mn(1) | 179.3(7) |
| C(2)-Mn(1)-C(3) | 88.8(3) | O(6)-C(6)-Mn(2) | 177.6(5) |
| C(1)-Mn(1)-C(5) | 94.4(4) | O(7)-C(7)-Mn(2) | 177.5(6) |
| C(4)-Mn(1)-C(5) | 91.5(3) | O(8)-C(8)-Mn(2) | 177.4(6) |
| C(2)-Mn(1)-C(5) | 89.7(3) | O(9)-C(9)-Mn(2) | 177.3(6) |
| C(3)-Mn(1)-C(5) | 169.9(3) | O(10)-C(10)-C(11) | 103.8(5) |
| C(1)-Mn(1)-Mn(2) | 177.8(3) | O(10)-C(10)-Mn(2) | 131.1(6) |
| C(4)-Mn(1)-Mn(2) | 84.6(2) | C(11)-C(10)-Mn(2) | 125.1(6) |
| C(2)-Mn(1)-Mn(2) | 85.85(19) | C(10)-O(10)-C(15) | 125.0(5) |
| C(3)-Mn(1)-Mn(2) | 86.2(2) | O(10)-C(15)-C(16) | 105.9(6) |
| C(5)-Mn(1)-Mn(2) | 83.7(2) | O(10)-C(15)-H(15A) | 110.6 |
| C(7)-Mn(2)-C(6) | 89.7(3) | C(16)-C(15)-H(15A) | 110.6 |
| C(7)-Mn(2)-C(8) | 88.5(3) | O(10)-C(15)-H(15B) | 110.5 |
| C(6)-Mn(2)-C(8) | 172.7(3) | C(16)-C(15)-H(15B) | 110.5 |
| C(7)-Mn(2)-C(9) | 171.8(3) | H(15A)-C(15)-H(15B) | 108.7 |
| C(6)-Mn(2)-C(9) | 87.2(3) | C(15)-C(16)-H(16A) | 109.5 |
| C(8)-Mn(2)-C(9) | 93.7(3) | C(15)-C(16)-H(16B) | 109.5 |
| C(7)-Mn(2)-C(10) | 96.5(4) | H(16A)-C(16)-H(16B) | 109.5 |
| C(6)-Mn(2)-C(10) | 95.7(4) | C(15)-C(16)-H(16C) | 109.5 |
| C(8)-Mn(2)-C(10) | 91.6(4) | H(16A)-C(16)-H(16C) | 109.5 |
| C(9)-Mn(2)-C(10) | 91.3(4) | H(16B)-C(16)-H(16C) | 109.5 |
| C(7)-Mn(2)-C(10A) | 98(2) | C(12)-C(11)-C(10) | 130.6(7) |
| C(6)-Mn(2)-C(10A) | 100(3) | C(12)-C(11)-S(1) | 109.0(6) |
| C(8)-Mn(2)-C(10A) | 87(3) | C(10)-C(11)-S(1) | 120.3(6) |

| | | | |
|---|---|---|---|
| C(14)-S(1)-C(11) | 92.3(5) | C(15A)-C(16A)-H(16D) | 109.5 |
| C(11)-C(12)-C(13) | 112.3(9) | C(15A)-C(16A)-H(16E) | 109.5 |
| C(11)-C(12)-H(12) | 123.8 | H(16D)-C(16A)-H(16E) | 109.5 |
| C(13)-C(12)-H(12) | 123.9 | C(15A)-C(16A)-H(16F) | 109.5 |
| C(14)-C(13)-C(12) | 114.0(9) | H(16D)-C(16A)-H(16F) | 109.5 |
| C(14)-C(13)-H(13) | 123.0 | H(16E)-C(16A)-H(16F) | 109.5 |
| C(12)-C(13)-H(13) | 123.0 | C(12A)-C(11A)-C(10A) | 130.5 |
| C(13)-C(14)-S(1) | 112.3(8) | C(12A)-C(11A)-S(1A) | 109.4 |
| C(13)-C(14)-H(14) | 123.9 | C(10A)-C(11A)-S(1A) | 120.1 |
| S(1)-C(14)-H(14) | 123.9 | C(14A)-S(1A)-C(11A) | 91.9 |
| O(10A)-C(10A)-C(11A) | 106.3 | C(11A)-C(12A)-C(13A) | 114.1 |
| O(10A)-C(10A)-Mn(2) | 133(3) | C(11A)-C(12A)-H(12A) | 123.0 |
| C(11A)-C(10A)-Mn(2) | 120(3) | C(13A)-C(12A)-H(12A) | 123.0 |
| C(10A)-O(10A)-C(15A) | 122.5 | C(14A)-C(13A)-C(12A) | 111.8 |
| O(10A)-C(15A)-C(16A) | 107.3 | C(14A)-C(13A)-H(13A) | 124.1 |
| O(10A)-C(15A)-H(15C) | 110.3 | C(12A)-C(13A)-H(13A) | 124.1 |
| C(16A)-C(15A)-H(15C) | 110.3 | C(13A)-C(14A)-S(1A) | 112.8 |
| O(10A)-C(15A)-H(15D) | 110.3 | C(13A)-C(14A)-H(14A) | 123.6 |
| C(16A)-C(15A)-H(15D) | 110.3 | S(1A)-C(14A)-H(14A) | 123.6 |
| H(15C)-C(15A)-H(15D) | 108.5 | | |

**Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)**

The anisotropic displacement factor exponent takes the form: $-2\pi^2[ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12} ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Mn(1) | 46(1) | 76(1) | 45(1) | -11(1) | -8(1) | 1(1) |
| Mn(2) | 39(1) | 52(1) | 39(1) | -5(1) | -4(1) | 3(1) |
| O(1) | 91(4) | 211(7) | 85(4) | -37(4) | -28(3) | -42(4) |
| O(2) | 87(4) | 82(3) | 66(3) | -11(2) | 18(3) | 13(3) |
| O(3) | 119(5) | 82(4) | 85(4) | 4(3) | 4(3) | -20(3) |
| O(4) | 52(3) | 175(6) | 97(4) | -34(4) | 11(3) | 10(4) |
| O(5) | 120(5) | 96(4) | 87(4) | 19(3) | -1(3) | 45(4) |
| O(6) | 107(4) | 77(3) | 81(4) | -6(3) | -1(3) | 46(3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O(7) | 72(3) | 108(4) | 57(3) | 0(3) | 11(2) | -18(3) |
| O(8) | 90(4) | 88(4) | 107(4) | -15(3) | -5(3) | 43(3) |
| O(9) | 85(3) | 89(3) | 59(3) | 4(2) | 16(3) | -12(3) |
| C(1) | 64(5) | 121(7) | 74(5) | -18(5) | -14(4) | -11(4) |
| C(2) | 64(4) | 62(4) | 47(4) | -7(3) | -4(3) | -2(3) |
| C(3) | 73(5) | 74(5) | 53(4) | -9(3) | -9(3) | -12(4) |
| C(4) | 45(4) | 117(6) | 61(5) | -18(4) | -5(3) | -2(4) |
| C(5) | 68(5) | 89(5) | 55(4) | -16(4) | -14(3) | 28(4) |
| C(6) | 60(4) | 61(4) | 43(4) | -4(3) | -3(3) | 2(3) |
| C(7) | 41(3) | 69(4) | 52(4) | -6(3) | -3(3) | -1(3) |
| C(8) | 61(4) | 70(4) | 49(4) | -6(3) | -2(3) | 7(3) |
| C(9) | 51(4) | 56(4) | 43(4) | -4(3) | 1(3) | 2(3) |
| C(10) | 38(4) | 53(5) | 42(4) | 3(3) | 6(3) | 3(3) |
| O(10) | 53(3) | 67(3) | 51(3) | 3(2) | -16(2) | -9(2) |
| C(11) | 59(6) | 60(6) | 42(5) | -14(3) | 6(3) | -11(3) |
| S(1) | 80(2) | 92(2) | 70(2) | -18(1) | -6(1) | -33(1) |
| C(12) | 114(9) | 59(6) | 46(5) | 0(4) | 2(4) | -22(5) |
| C(13) | 180(15) | 59(6) | 74(8) | -2(5) | 44(8) | -32(7) |
| C(14) | 133(9) | 81(6) | 85(8) | -22(5) | 19(6) | -58(6) |
| C(15) | 69(6) | 79(5) | 55(5) | 22(4) | -18(4) | -6(4) |
| C(16) | 75(7) | 114(7) | 93(8) | 48(6) | -35(6) | -16(6) |

**Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$)**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(12) | 410 | 4713 | 3019 | 88 |
| H(13) | -1237 | 3807 | 2680 | 123 |
| H(14) | -3488 | 3908 | 1226 | 119 |
| H(15A) | 51 | 6596 | -209 | 83 |
| H(15B) | -1123 | 6841 | 712 | 83 |
| H(16A) | -2399 | 6995 | -1182 | 145 |
| H(16B) | -3513 | 6566 | -493 | 145 |
| H(16C) | -2366 | 6299 | -1400 | 145 |
| H(12A) | -40 | 6785 | 351 | 97 |

| | | | | |
|---|---|---|---|---|
| H(13A) | -1983 | 7006 | -1364 | 97 |
| H(14A) | -3939 | 6191 | -1847 | 97 |
| H(15C) | -554 | 4880 | 3302 | 63 |
| H(15D) | 736 | 4595 | 2505 | 63 |
| H(16D) | -1238 | 3866 | 2956 | 79 |
| H(16E) | -1440 | 3988 | 1612 | 79 |
| H(16F) | -2724 | 4272 | 2407 | 79 |

**Table 6. Torsion angles [°]**

| | | | |
|---|---|---|---|
| C(4)-Mn(1)-Mn(2)-C(7) | -44.7(3) | C(9)-Mn(2)-C(10)-O(10) | 132.7(9) |
| C(2)-Mn(1)-Mn(2)-C(7) | 133.0(3) | C(6)-Mn(2)-C(10)-C(11) | -132.0(6) |
| C(3)-Mn(1)-Mn(2)-C(7) | 43.9(3) | C(7)-Mn(2)-C(10)-C(11) | 137.6(6) |
| C(5)-Mn(1)-Mn(2)-C(7) | -136.8(3) | C(8)-Mn(2)-C(10)-C(11) | 48.9(7) |
| C(4)-Mn(1)-Mn(2)-C(6) | -134.6(3) | C(9)-Mn(2)-C(10)-C(11) | -44.8(7) |
| C(2)-Mn(1)-Mn(2)-C(6) | 43.1(3) | C(11)-C(10)-O(10)-C(15) | 177.2(8) |
| C(3)-Mn(1)-Mn(2)-C(6) | -46.0(3) | Mn(2)-C(10)-O(10)-C(15) | -0.7(16) |
| C(5)-Mn(1)-Mn(2)-C(6) | 133.3(3) | C(10)-O(10)-C(15)-C(16) | -169.7(7) |
| C(4)-Mn(1)-Mn(2)-C(8) | 44.0(3) | O(10)-C(10)-C(11)-C(12) | 175.5(9) |
| C(2)-Mn(1)-Mn(2)-C(8) | -138.3(3) | Mn(2)-C(10)-C(11)-C(12) | -6.4(11) |
| C(3)-Mn(1)-Mn(2)-C(8) | 132.7(3) | O(10)-C(10)-C(11)-S(1) | -7.1(9) |
| C(5)-Mn(1)-Mn(2)-C(8) | -48.1(3) | Mn(2)-C(10)-C(11)-S(1) | 171.0(10) |
| C(4)-Mn(1)-Mn(2)-C(9) | 138.0(3) | C(12)-C(11)-S(1)-C(14) | 0.1(7) |
| C(2)-Mn(1)-Mn(2)-C(9) | -44.3(3) | C(10)-C(11)-S(1)-C(14) | -177.8(8) |
| C(3)-Mn(1)-Mn(2)-C(9) | -133.4(3) | C(10)-C(11)-C(12)-C(13) | 179.6(9) |
| C(5)-Mn(1)-Mn(2)-C(9) | 45.9(3) | S(1)-C(11)-C(12)-C(13) | 1.9(10) |
| C(7)-Mn(2)-C(10)-O(10) | -44.9(10) | C(11)-C(12)-C(13)-C(14) | -3.7(15) |
| C(6)-Mn(2)-C(10)-O(10) | 45.5(10) | C(12)-C(13)-C(14)-S(1) | 3.7(15) |
| C(8)-Mn(2)-C(10)-O(10) | -133.6(9) | C(11)-S(1)-C(14)-C(13) | -2.2(10) |

# Appendix 2

## Crystallographic data of Complex 3

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

| | | |
|---|---|---|
| Identification code | DBMCO2 | |
| Empirical formula | $C_{16}$ $H_8$ $Mn_2$ $O_{11}$ | |
| Formula weight | 486.10 | |
| Temperature | 293(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P $2_1$/c | |
| Unit cell dimensions | a = 12.4868(14) Å | α = 90°. |
| | b = 12.3976(14) Å | β = 92.723(2)°. |
| | c = 12.5593(14) Å | γ = 90°. |
| Volume | 1942.1(4) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.663 $Mg/m^3$ | |
| Absorption coefficient | 1.357 $mm^{-1}$ | |
| F(000) | 968 | |
| Crystal size | 0.36 x 0.23 x 0.18 $mm^3$ | |
| Theta range for data collection | 2.31 to 26.47°. | |
| Index ranges | -15<=h<=15, -15<=k<=14, -4<=l<=15 | |
| Reflections collected | 10177 | |
| Independent reflections | 3652 [R(int) = 0.0216] | |
| Completeness to theta = 25.00° | 99.4 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.783 and 0.715 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3652 / 0 / 294 | |
| Goodness-of-fit on $F^2$ | 1.083 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0303, wR2 = 0.0771 | |
| R indices (all data) | R1 = 0.0385, wR2 = 0.0846 | |
| Extinction coefficient | 0 | |
| Largest diff. peak and hole | 0.307 and -0.191 $e.Å^{-3}$ | |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Mn(1) | 1030(1) | 1423(1) | 3219(1) | 48(1) |
| Mn(2) | 2905(1) | 371(1) | 2358(1) | 47(1) |
| C(1) | -62(2) | 2125(2) | 3822(2) | 63(1) |
| O(1) | -728(2) | 2571(2) | 4217(2) | 92(1) |
| C(2) | 1238(2) | 476(2) | 4343(2) | 56(1) |
| O(2) | 1338(2) | -95(2) | 5045(1) | 78(1) |
| C(3) | 2037(2) | 2335(2) | 3838(2) | 60(1) |
| O(3) | 2635(2) | 2916(2) | 4240(2) | 91(1) |
| C(4) | 993(2) | 2266(2) | 2008(2) | 64(1) |
| O(4) | 954(2) | 2805(2) | 1275(2) | 99(1) |
| C(5) | 165(2) | 409(2) | 2512(2) | 65(1) |
| O(5) | -382(2) | -208(2) | 2093(2) | 98(1) |
| C(6) | 3508(2) | 479(2) | 3718(2) | 56(1) |
| O(6) | 3850(2) | 525(2) | 4577(1) | 77(1) |
| C(7) | 3369(2) | 1735(2) | 2020(2) | 60(1) |
| O(7) | 3650(2) | 2580(2) | 1802(2) | 86(1) |
| C(8) | 2082(2) | 321(2) | 1088(2) | 59(1) |
| O(8) | 1564(2) | 277(2) | 326(1) | 85(1) |
| C(9) | 2254(2) | -900(2) | 2725(2) | 55(1) |
| O(9) | 1844(2) | -1685(2) | 2956(1) | 75(1) |
| C(10) | 4104(2) | -354(2) | 1753(2) | 55(1) |
| O(10) | 5158(1) | -187(2) | 1863(1) | 74(1) |
| C(11) | 4018(2) | -1257(2) | 1025(2) | 57(1) |
| O(11) | 3019(1) | -1702(2) | 812(1) | 77(1) |
| C(12) | 4723(2) | -1811(2) | 450(2) | 76(1) |
| C(13) | 4157(2) | -2614(2) | -127(2) | 81(1) |
| C(14) | 3147(3) | -2525(2) | 116(2) | 81(1) |
| C(15) | 5651(2) | 634(4) | 2539(4) | 89(1) |
| C(16) | 6825(3) | 541(4) | 2424(4) | 100(1) |

**Table 3. Bond lengths [Å] and angles [°]**

| | | | |
|---|---|---|---|
| Mn(1)-C(1) | 1.813(2) | C(16)-H(16A) | 0.82(4) |
| Mn(1)-C(3) | 1.836(3) | C(16)-H(16B) | 0.92(4) |
| Mn(1)-C(4) | 1.844(2) | C(16)-H(16C) | 0.92(5) |
| Mn(1)-C(2) | 1.845(2) | | |
| Mn(1)-C(5) | 1.857(3) | C(1)-Mn(1)-C(3) | 92.36(11) |
| Mn(1)-Mn(2) | 2.9316(5) | C(1)-Mn(1)-C(4) | 94.76(10) |
| Mn(2)-C(6) | 1.839(2) | C(3)-Mn(1)-C(4) | 89.46(11) |
| Mn(2)-C(9) | 1.842(2) | C(1)-Mn(1)-C(2) | 93.81(10) |
| Mn(2)-C(7) | 1.844(3) | C(3)-Mn(1)-C(2) | 89.98(10) |
| Mn(2)-C(8) | 1.857(2) | C(4)-Mn(1)-C(2) | 171.43(10) |
| Mn(2)-C(10) | 1.932(2) | C(1)-Mn(1)-C(5) | 95.33(11) |
| C(1)-O(1) | 1.133(3) | C(3)-Mn(1)-C(5) | 172.32(10) |
| C(2)-O(2) | 1.133(3) | C(4)-Mn(1)-C(5) | 89.87(11) |
| C(3)-O(3) | 1.138(3) | C(2)-Mn(1)-C(5) | 89.54(11) |
| C(4)-O(4) | 1.136(3) | C(1)-Mn(1)-Mn(2) | 175.74(8) |
| C(5)-O(5) | 1.137(3) | C(3)-Mn(1)-Mn(2) | 83.55(7) |
| C(6)-O(6) | 1.142(3) | C(4)-Mn(1)-Mn(2) | 86.40(8) |
| C(7)-O(7) | 1.142(3) | C(2)-Mn(1)-Mn(2) | 85.04(7) |
| C(8)-O(8) | 1.130(3) | C(5)-Mn(1)-Mn(2) | 88.77(8) |
| C(9)-O(9) | 1.144(3) | C(6)-Mn(2)-C(9) | 89.74(9) |
| C(10)-O(10) | 1.332(3) | C(6)-Mn(2)-C(7) | 91.61(10) |
| C(10)-C(11) | 1.446(3) | C(9)-Mn(2)-C(7) | 171.74(10) |
| O(10)-C(15) | 1.444(3) | C(6)-Mn(2)-C(8) | 170.35(10) |
| C(11)-C(12) | 1.352(3) | C(9)-Mn(2)-C(8) | 87.33(9) |
| C(11)-O(11) | 1.379(3) | C(7)-Mn(2)-C(8) | 90.02(10) |
| O(11)-C(14) | 1.358(3) | C(6)-Mn(2)-C(10) | 96.22(9) |
| C(12)-C(13) | 1.403(4) | C(9)-Mn(2)-C(10) | 93.42(9) |
| C(12)-H(12) | 0.94(3) | C(7)-Mn(2)-C(10) | 94.53(10) |
| C(13)-C(14) | 1.317(4) | C(8)-Mn(2)-C(10) | 93.14(9) |
| C(13)-H(13) | 1.01(4) | C(6)-Mn(2)-Mn(1) | 85.62(7) |
| C(14)-H(14) | 1.03(3) | C(9)-Mn(2)-Mn(1) | 85.33(7) |
| C(15)-C(16) | 1.484(5) | C(7)-Mn(2)-Mn(1) | 86.64(7) |
| C(15)-H(15A) | 0.86(3) | C(8)-Mn(2)-Mn(1) | 84.98(7) |
| C(15)-H(15B) | 0.86(3) | C(10)-Mn(2)-Mn(1) | 177.78(7) |

| | | | |
|---|---|---|---|
| O(1)-C(1)-Mn(1) | 178.4(2) | C(13)-C(12)-H(12) | 125.0(19) |
| O(2)-C(2)-Mn(1) | 178.0(2) | C(14)-C(13)-C(12) | 106.6(2) |
| O(3)-C(3)-Mn(1) | 177.7(2) | C(14)-C(13)-H(13) | 129.7(19) |
| O(4)-C(4)-Mn(1) | 178.2(2) | C(12)-C(13)-H(13) | 123.7(19) |
| O(5)-C(5)-Mn(1) | 178.5(2) | C(13)-C(14)-O(11) | 110.8(3) |
| O(6)-C(6)-Mn(2) | 177.4(2) | C(13)-C(14)-H(14) | 135.2(18) |
| O(7)-C(7)-Mn(2) | 179.3(2) | O(11)-C(14)-H(14) | 113.5(18) |
| O(8)-C(8)-Mn(2) | 178.5(2) | O(10)-C(15)-C(16) | 106.5(3) |
| O(9)-C(9)-Mn(2) | 179.5(2) | O(10)-C(15)-H(15A) | 114(2) |
| O(10)-C(10)-C(11) | 103.25(18) | C(16)-C(15)-H(15A) | 118(2) |
| O(10)-C(10)-Mn(2) | 131.79(16) | O(10)-C(15)-H(15B) | 111(2) |
| C(11)-C(10)-Mn(2) | 124.96(15) | C(16)-C(15)-H(15B) | 115(2) |
| C(10)-O(10)-C(15) | 124.2(2) | H(15A)-C(15)-H(15B) | 93(3) |
| C(12)-C(11)-O(11) | 107.4(2) | C(15)-C(16)-H(16A) | 112(3) |
| C(12)-C(11)-C(10) | 134.4(2) | C(15)-C(16)-H(16B) | 108(3) |
| O(11)-C(11)-C(10) | 118.13(18) | H(16A)-C(16)-H(16B) | 119(4) |
| C(14)-O(11)-C(11) | 107.0(2) | C(15)-C(16)-H(16C) | 115(3) |
| C(11)-C(12)-C(13) | 108.2(2) | H(16A)-C(16)-H(16C) | 101(4) |
| C(11)-C(12)-H(12) | 126.7(19) | H(16B)-C(16)-H(16C) | 103(4) |

**Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)**

The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Mn(1) | 43(1) | 55(1) | 46(1) | 5(1) | 7(1) | 4(1) |
| Mn(2) | 45(1) | 52(1) | 46(1) | -2(1) | 6(1) | 1(1) |
| C(1) | 53(1) | 74(2) | 63(1) | 13(1) | 10(1) | 11(1) |
| O(1) | 70(1) | 107(2) | 103(1) | 13(1) | 30(1) | 37(1) |
| C(2) | 48(1) | 63(1) | 57(1) | 5(1) | 11(1) | 5(1) |
| O(2) | 81(1) | 87(1) | 68(1) | 29(1) | 14(1) | 12(1) |
| C(3) | 52(1) | 65(1) | 63(1) | -4(1) | 15(1) | 5(1) |
| O(3) | 68(1) | 95(1) | 109(1) | -39(1) | 12(1) | -14(1) |
| C(4) | 69(2) | 66(1) | 58(1) | 7(1) | 10(1) | 6(1) |
| O(4) | 131(2) | 97(1) | 70(1) | 35(1) | 13(1) | 21(1) |
| C(5) | 52(1) | 77(2) | 67(1) | 6(1) | 2(1) | 0(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O(5) | 77(1) | 107(2) | 108(2) | -9(1) | -15(1) | -26(1) |
| C(6) | 48(1) | 61(1) | 60(1) | -2(1) | 6(1) | 2(1) |
| O(6) | 69(1) | 101(1) | 60(1) | -3(1) | -8(1) | 2(1) |
| C(7) | 55(1) | 63(1) | 62(1) | -5(1) | 16(1) | 2(1) |
| O(7) | 89(1) | 64(1) | 107(1) | 6(1) | 30(1) | -8(1) |
| C(8) | 61(1) | 64(1) | 52(1) | 5(1) | 8(1) | 0(1) |
| O(8) | 94(1) | 100(2) | 59(1) | 7(1) | -16(1) | -5(1) |
| C(9) | 56(1) | 62(1) | 46(1) | -2(1) | 2(1) | 4(1) |
| O(9) | 91(1) | 65(1) | 69(1) | 6(1) | 6(1) | -14(1) |
| C(10) | 47(1) | 61(1) | 57(1) | -4(1) | 4(1) | -2(1) |
| O(10) | 46(1) | 88(1) | 88(1) | -28(1) | 4(1) | -3(1) |
| C(11) | 48(1) | 64(1) | 60(1) | -10(1) | 7(1) | 2(1) |
| O(11) | 59(1) | 89(1) | 84(1) | -37(1) | 14(1) | -13(1) |
| C(12) | 57(2) | 82(2) | 91(2) | -21(2) | 11(1) | 6(1) |
| C(13) | 82(2) | 76(2) | 86(2) | -27(2) | 12(2) | 5(1) |
| C(14) | 80(2) | 86(2) | 79(2) | -34(2) | 16(1) | -14(2) |
| C(15) | 55(2) | 105(3) | 108(3) | -42(2) | 3(2) | -13(2) |
| C(16) | 54(2) | 111(3) | 133(3) | -31(3) | -3(2) | -12(2) |

**Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$x $10^3$)**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(12) | 5460(30) | -1670(20) | 410(20) | 94(9) |
| H(13) | 4510(30) | -3150(30) | -610(30) | 110(11) |
| H(14) | 2440(30) | -2870(30) | -150(20) | 101(10) |
| H(15A) | 5360(20) | 1260(30) | 2450(20) | 78(10) |
| H(15B) | 5450(30) | 580(30) | 3180(30) | 96(11) |
| H(16A) | 7160(30) | 1000(30) | 2780(30) | 112(13) |
| H(16B) | 6950(30) | 480(30) | 1710(30) | 119(14) |
| H(16C) | 7130(40) | -80(50) | 2700(40) | 170(20) |

**Table 6. Torsion angles [°]**

| | | | |
|---|---|---|---|
| C(3)-Mn(1)-Mn(2)-C(6) | 45.97(10) | C(4)-Mn(1)-Mn(2)-C(6) | 135.84(11) |

| | | | |
|---|---|---|---|
| C(2)-Mn(1)-Mn(2)-C(6) | -44.57(10) | C(2)-Mn(1)-Mn(2)-C(8) | 133.24(10) |
| C(5)-Mn(1)-Mn(2)-C(6) | -134.21(10) | C(5)-Mn(1)-Mn(2)-C(8) | 43.60(10) |
| C(3)-Mn(1)-Mn(2)-C(9) | 136.07(10) | C(6)-Mn(2)-C(10)-O(10) | -43.4(2) |
| C(4)-Mn(1)-Mn(2)-C(9) | -134.07(10) | C(9)-Mn(2)-C(10)-O(10) | -133.5(2) |
| C(2)-Mn(1)-Mn(2)-C(9) | 45.52(9) | C(7)-Mn(2)-C(10)-O(10) | 48.7(2) |
| C(5)-Mn(1)-Mn(2)-C(9) | -44.12(10) | C(8)-Mn(2)-C(10)-O(10) | 139.0(2) |
| C(3)-Mn(1)-Mn(2)-C(7) | -45.90(11) | C(6)-Mn(2)-C(10)-C(11) | 137.1(2) |
| C(4)-Mn(1)-Mn(2)-C(7) | 43.97(11) | C(9)-Mn(2)-C(10)-C(11) | 47.0(2) |
| C(2)-Mn(1)-Mn(2)-C(7) | -136.44(10) | C(7)-Mn(2)-C(10)-C(11) | -130.8(2) |
| C(5)-Mn(1)-Mn(2)-C(7) | 133.91(11) | C(8)-Mn(2)-C(10)-C(11) | -40.5(2) |
| C(3)-Mn(1)-Mn(2)-C(8) | -136.21(10) | C(11)-C(10)-O(10)-C(15) | -178.9(3) |
| C(4)-Mn(1)-Mn(2)-C(8) | -46.35(11) | | |

# Appendix 3

## Crystallographic data of Complex 5

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

| | | |
|---|---|---|
| Identification code | dbmc12_abs | |
| Empirical formula | $C_{16}$ $H_8$ $O_{11}$ $Re_2$ | |
| Formula weight | 748.62 | |
| Temperature | 293(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Orthorhombic | |
| Space group | P b c a | |
| Unit cell dimensions | a = 12.9646(8) Å | α = 90º. |
| | b = 15.6580(9) Å | β = 90º. |
| | c = 19.3844(11) Å | γ = 90º. |
| Volume | 3935.0(4) $Å^3$ | |
| Z | 8 | |
| Density (calculated) | 2.527 $Mg/m^3$ | |
| Absorption coefficient | 12.350 $mm^{-1}$ | |
| F(000) | 2736 | |
| Crystal size | 0.34 x 0.22 x 0.20 $mm^3$ | |
| Theta range for data collection | 2.60 to 26.58º. | |
| Index ranges | -16<=h<=16, -14<=k<=18, -24<=l<=12 | |
| Reflections collected | 20120 | |
| Independent reflections | 3784 [R(int) = 0.0346] | |
| Completeness to theta = 25.00º | 99.9 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.085 and 0.045 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3784 / 0 / 263 | |
| Goodness-of-fit on $F^2$ | 1.134 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0205, wR2 = 0.0506 | |
| R indices (all data) | R1 = 0.0229, wR2 = 0.0520 | |
| Extinction coefficient | 0.00093(4) | |
| Largest diff. peak and hole | 0.927 and -0.651 e.$Å^{-3}$ | |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Re(1) | 4861(1) | 2119(1) | 6807(1) | 35(1) |
| Re(2) | 4325(1) | 1913(1) | 5268(1) | 37(1) |
| C(1) | 5279(3) | 2230(3) | 7755(2) | 51(1) |
| O(1) | 5535(3) | 2252(3) | 8314(2) | 73(1) |
| C(2) | 6290(3) | 2254(2) | 6454(2) | 41(1) |
| O(2) | 7119(2) | 2207(2) | 6257(2) | 60(1) |
| C(3) | 5220(4) | 883(3) | 6841(2) | 49(1) |
| O(3) | 5434(4) | 194(2) | 6877(2) | 84(1) |
| C(4) | 3463(3) | 1722(3) | 7087(2) | 48(1) |
| O(4) | 2729(2) | 1401(2) | 7259(2) | 68(1) |
| C(5) | 4015(3) | 1667(3) | 4312(2) | 48(1) |
| O(5) | 3848(3) | 1509(2) | 3753(2) | 66(1) |
| C(6) | 3282(4) | 2844(3) | 5347(2) | 49(1) |
| O(6) | 2694(3) | 3372(3) | 5370(2) | 78(1) |
| C(7) | 5399(4) | 2777(3) | 5027(2) | 47(1) |
| O(7) | 5994(3) | 3271(3) | 4880(2) | 76(1) |
| C(8) | 5414(3) | 1027(3) | 5312(2) | 48(1) |
| O(8) | 6039(3) | 514(2) | 5328(2) | 67(1) |
| C(9) | 3282(3) | 1082(3) | 5600(2) | 47(1) |
| O(9) | 2664(3) | 607(2) | 5770(2) | 73(1) |
| C(10) | 4491(3) | 3432(2) | 6664(2) | 37(1) |
| O(10) | 3616(2) | 3846(2) | 6771(1) | 48(1) |
| C(11) | 5188(3) | 4102(3) | 6431(2) | 44(1) |
| O(11) | 6210(2) | 3927(2) | 6334(2) | 60(1) |
| C(12) | 5017(4) | 4937(3) | 6285(3) | 67(1) |
| C(13) | 5978(4) | 5302(4) | 6097(3) | 83(2) |
| C(14) | 6664(4) | 4671(3) | 6137(3) | 77(2) |
| C(15) | 2693(3) | 3457(3) | 7043(2) | 50(1) |
| C(16) | 1883(4) | 4144(3) | 7027(3) | 80(2) |

**Table 3. Bond lengths [Å] and angles [º]**

| | | | |
|---|---|---|---|
| Re(1)-C(1) | 1.923(5) | C(16)-H(16B) | 0.9600 |
| Re(1)-C(2) | 1.987(4) | C(16)-H(16C) | 0.9600 |
| Re(1)-C(4) | 1.992(4) | | |
| Re(1)-C(3) | 1.992(5) | C(1)-Re(1)-C(2) | 93.26(18) |
| Re(1)-C(10) | 2.129(4) | C(1)-Re(1)-C(4) | 91.36(19) |
| Re(1)-Re(2) | 3.0809(3) | C(2)-Re(1)-C(4) | 167.42(16) |
| Re(2)-C(5) | 1.934(4) | C(1)-Re(1)-C(3) | 89.42(19) |
| Re(2)-C(8) | 1.981(5) | C(2)-Re(1)-C(3) | 84.07(17) |
| Re(2)-C(9) | 1.984(4) | C(4)-Re(1)-C(3) | 84.28(17) |
| Re(2)-C(6) | 1.995(5) | C(1)-Re(1)-C(10) | 95.82(17) |
| Re(2)-C(7) | 1.997(4) | C(2)-Re(1)-C(10) | 93.60(15) |
| C(1)-O(1) | 1.135(5) | C(4)-Re(1)-C(10) | 97.58(15) |
| C(2)-O(2) | 1.143(5) | C(3)-Re(1)-C(10) | 174.38(15) |
| C(3)-O(3) | 1.117(6) | C(1)-Re(1)-Re(2) | 176.58(13) |
| C(4)-O(4) | 1.127(5) | C(2)-Re(1)-Re(2) | 83.56(11) |
| C(5)-O(5) | 1.132(5) | C(4)-Re(1)-Re(2) | 91.50(13) |
| C(6)-O(6) | 1.126(5) | C(3)-Re(1)-Re(2) | 89.00(12) |
| C(7)-O(7) | 1.128(6) | C(10)-Re(1)-Re(2) | 85.66(9) |
| C(8)-O(8) | 1.141(5) | C(5)-Re(2)-C(8) | 92.90(17) |
| C(9)-O(9) | 1.142(5) | C(5)-Re(2)-C(9) | 92.26(17) |
| C(10)-O(10) | 1.323(5) | C(8)-Re(2)-C(9) | 90.72(18) |
| C(10)-C(11) | 1.457(5) | C(5)-Re(2)-C(6) | 94.52(17) |
| O(10)-C(15) | 1.443(5) | C(8)-Re(2)-C(6) | 172.56(17) |
| C(11)-C(12) | 1.355(6) | C(9)-Re(2)-C(6) | 89.60(18) |
| C(11)-O(11) | 1.367(5) | C(5)-Re(2)-C(7) | 93.18(17) |
| O(11)-C(14) | 1.360(5) | C(8)-Re(2)-C(7) | 89.3(2) |
| C(12)-C(13) | 1.418(7) | C(9)-Re(2)-C(7) | 174.55(17) |
| C(12)-H(12) | 0.9300 | C(6)-Re(2)-C(7) | 89.7(2) |
| C(13)-C(14) | 1.331(8) | C(5)-Re(2)-Re(1) | 174.48(13) |
| C(13)-H(13) | 0.9300 | C(8)-Re(2)-Re(1) | 82.54(12) |
| C(14)-H(14) | 0.9300 | C(9)-Re(2)-Re(1) | 84.71(12) |
| C(15)-C(16) | 1.504(6) | C(6)-Re(2)-Re(1) | 90.08(12) |
| C(15)-H(15A) | 0.9700 | C(7)-Re(2)-Re(1) | 89.89(12) |
| C(15)-H(15B) | 0.9700 | O(1)-C(1)-Re(1) | 176.6(4) |
| C(16)-H(16A) | 0.9600 | O(2)-C(2)-Re(1) | 170.1(3) |

| | | | |
|---|---|---|---|
| O(3)-C(3)-Re(1) | 178.1(5) | C(14)-C(13)-C(12) | 105.9(5) |
| O(4)-C(4)-Re(1) | 171.4(4) | C(14)-C(13)-H(13) | 127.1 |
| O(5)-C(5)-Re(2) | 178.6(4) | C(12)-C(13)-H(13) | 127.1 |
| O(6)-C(6)-Re(2) | 177.9(4) | C(13)-C(14)-O(11) | 111.2(4) |
| O(7)-C(7)-Re(2) | 178.7(4) | C(13)-C(14)-H(14) | 124.4 |
| O(8)-C(8)-Re(2) | 179.0(4) | O(11)-C(14)-H(14) | 124.4 |
| O(9)-C(9)-Re(2) | 177.5(4) | O(10)-C(15)-C(16) | 105.6(3) |
| O(10)-C(10)-C(11) | 103.1(3) | O(10)-C(15)-H(15A) | 110.6 |
| O(10)-C(10)-Re(1) | 130.2(3) | C(16)-C(15)-H(15A) | 110.6 |
| C(11)-C(10)-Re(1) | 126.6(3) | O(10)-C(15)-H(15B) | 110.6 |
| C(10)-O(10)-C(15) | 124.1(3) | C(16)-C(15)-H(15B) | 110.6 |
| C(12)-C(11)-O(11) | 108.9(4) | H(15A)-C(15)-H(15B) | 108.7 |
| C(12)-C(11)-C(10) | 131.2(4) | C(15)-C(16)-H(16A) | 109.5 |
| O(11)-C(11)-C(10) | 119.9(3) | C(15)-C(16)-H(16B) | 109.5 |
| C(14)-O(11)-C(11) | 106.6(4) | H(16A)-C(16)-H(16B) | 109.5 |
| C(11)-C(12)-C(13) | 107.4(5) | C(15)-C(16)-H(16C) | 109.5 |
| C(11)-C(12)-H(12) | 126.3 | H(16A)-C(16)-H(16C) | 109.5 |
| C(13)-C(12)-H(12) | 126.3 | H(16B)-C(16)-H(16C) | 109.5 |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Re(1) | 38(1) | 31(1) | 35(1) | 0(1) | 2(1) | 0(1) |
| Re(2) | 38(1) | 35(1) | 37(1) | 1(1) | -2(1) | -1(1) |
| C(1) | 52(3) | 55(3) | 45(2) | -1(2) | 2(2) | 3(2) |
| O(1) | 84(3) | 95(3) | 41(2) | -3(2) | -9(2) | 6(2) |
| C(2) | 41(2) | 37(2) | 44(2) | -2(2) | 1(2) | 0(2) |
| O(2) | 42(2) | 63(2) | 75(2) | 0(2) | 7(2) | 1(1) |
| C(3) | 55(3) | 43(3) | 50(3) | 1(2) | 9(2) | 4(2) |
| O(3) | 106(3) | 36(2) | 109(3) | 10(2) | 19(2) | 18(2) |
| C(4) | 51(2) | 35(2) | 58(2) | -1(2) | 12(2) | 5(2) |
| O(4) | 54(2) | 48(2) | 101(2) | 9(2) | 27(2) | -6(2) |
| C(5) | 45(2) | 44(2) | 55(3) | -4(2) | -3(2) | -2(2) |
| O(5) | 78(2) | 73(2) | 47(2) | -16(2) | -12(2) | -2(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(6) | 54(3) | 50(2) | 45(2) | 0(2) | -7(2) | 5(2) |
| O(6) | 84(3) | 74(2) | 75(2) | -10(2) | -16(2) | 35(2) |
| C(7) | 56(2) | 47(2) | 39(2) | 1(2) | -2(2) | -9(2) |
| O(7) | 84(2) | 75(2) | 68(2) | 8(2) | 9(2) | -35(2) |
| C(8) | 44(2) | 45(2) | 53(2) | -3(2) | -4(2) | -2(2) |
| O(8) | 56(2) | 55(2) | 89(3) | -8(2) | 2(2) | 14(2) |
| C(9) | 45(2) | 47(2) | 49(2) | 8(2) | -1(2) | 3(2) |
| O(9) | 63(2) | 67(2) | 89(3) | 23(2) | 2(2) | -17(2) |
| C(10) | 43(2) | 32(2) | 35(2) | -2(1) | -1(2) | -2(2) |
| O(10) | 47(2) | 35(2) | 62(2) | 3(1) | 11(1) | 2(1) |
| C(11) | 42(2) | 36(2) | 55(2) | -5(2) | 2(2) | -4(2) |
| O(11) | 46(2) | 42(2) | 92(2) | -3(2) | 13(2) | -7(1) |
| C(12) | 62(3) | 43(3) | 96(4) | 21(3) | 4(3) | 0(2) |
| C(13) | 75(3) | 56(3) | 120(5) | 24(3) | 13(3) | -21(3) |
| C(14) | 62(3) | 49(3) | 119(5) | 5(3) | 24(3) | -21(2) |
| C(15) | 49(2) | 41(2) | 61(2) | 10(2) | 16(2) | 5(2) |
| C(16) | 64(3) | 52(3) | 123(5) | 25(3) | 42(3) | 18(2) |

**Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$x $10^3$)**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(12) | 4386 | 5218 | 6305 | 80 |
| H(13) | 6103 | 5866 | 5972 | 100 |
| H(14) | 7363 | 4732 | 6041 | 92 |
| H(15A) | 2805 | 3260 | 7512 | 60 |
| H(15B) | 2486 | 2974 | 6761 | 60 |
| H(16A) | 2014 | 4522 | 6647 | 120 |
| H(16B) | 1902 | 4461 | 7451 | 120 |
| H(16C) | 1215 | 3888 | 6972 | 120 |

**Table 6. Torsion angles [º]**

| | | | |
|---|---|---|---|
| C(2)-Re(1)-Re(2)-C(8) | 53.22(17) | C(10)-Re(1)-Re(2)-C(8) | 147.34(16) |
| C(4)-Re(1)-Re(2)-C(8) | -115.18(17) | C(2)-Re(1)-Re(2)-C(9) | 144.64(16) |
| C(3)-Re(1)-Re(2)-C(8) | -30.93(19) | C(4)-Re(1)-Re(2)-C(9) | -23.76(16) |

| | |
|---|---|
| C(3)-Re(1)-Re(2)-C(9) | 60.49(17) |
| C(10)-Re(1)-Re(2)-C(9) | -121.24(16) |
| C(2)-Re(1)-Re(2)-C(6) | -125.77(18) |
| C(4)-Re(1)-Re(2)-C(6) | 65.83(18) |
| C(3)-Re(1)-Re(2)-C(6) | 150.08(19) |
| C(10)-Re(1)-Re(2)-C(6) | -31.65(17) |
| C(2)-Re(1)-Re(2)-C(7) | -36.09(18) |
| C(4)-Re(1)-Re(2)-C(7) | 155.52(18) |
| C(3)-Re(1)-Re(2)-C(7) | -120.24(19) |
| C(10)-Re(1)-Re(2)-C(7) | 58.03(17) |
| C(1)-Re(1)-C(10)-O(10) | -88.6(4) |
| C(2)-Re(1)-C(10)-O(10) | 177.7(3) |
| C(4)-Re(1)-C(10)-O(10) | 3.5(4) |
| Re(2)-Re(1)-C(10)-O(10) | 94.5(3) |
| C(1)-Re(1)-C(10)-C(11) | 89.7(3) |
| C(2)-Re(1)-C(10)-C(11) | -3.9(3) |
| C(4)-Re(1)-C(10)-C(11) | -178.1(3) |
| Re(2)-Re(1)-C(10)-C(11) | -87.2(3) |
| C(11)-C(10)-O(10)-C(15) | -176.7(4) |
| Re(1)-C(10)-O(10)-C(15) | 1.9(5) |
| O(10)-C(10)-C(11)-C(12) | -5.7(6) |
| Re(1)-C(10)-C(11)-C(12) | 175.6(4) |
| O(10)-C(10)-C(11)-O(11) | 173.3(4) |
| Re(1)-C(10)-C(11)-O(11) | -5.4(5) |
| C(12)-C(11)-O(11)-C(14) | 0.8(5) |
| C(10)-C(11)-O(11)-C(14) | -178.4(4) |
| O(11)-C(11)-C(12)-C(13) | -0.6(6) |
| C(10)-C(11)-C(12)-C(13) | 178.5(5) |
| C(11)-C(12)-C(13)-C(14) | 0.3(7) |
| C(12)-C(13)-C(14)-O(11) | 0.2(7) |
| C(11)-O(11)-C(14)-C(13) | -0.6(6) |
| C(10)-O(10)-C(15)-C(16) | -175.9(4) |

# Appendix 4

## Crystallographic data of Complex 7

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

| | | |
|---|---|---|
| Identification code | db14d_absd | |
| Empirical formula | $C_{11}$ $H_8$ I Mn $O_5$ S | |
| Formula weight | 434.07 | |
| Temperature | 293(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Tetragonal | |
| Space group | I $4_1$/a | |
| Unit cell dimensions | a = 21.438(8) Å | α = 90°. |
| | b = 21.438(8) Å | β = 90°. |
| | c = 12.895(10) Å | γ = 90°. |
| Volume | 5926(5) $Å^3$ | |
| Z | 16 | |
| Density (calculated) | 1.946 $Mg/m^3$ | |
| Absorption coefficient | 3.125 $mm^{-1}$ | |
| F(000) | 3328 | |
| Crystal size | 0.58 x 0.54 x 0.42 $mm^3$ | |
| Theta range for data collection | 2.65 to 26.43°. | |
| Index ranges | -25<=h<=21, -20<=k<=25, -15<=l<=10 | |
| Reflections collected | 11926 | |
| Independent reflections | 2678 [R(int) = 0.0339] | |
| Completeness to theta = 25.00° | 93.1 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.269 and 0.188 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 2678 / 0 / 181 | |
| Goodness-of-fit on $F^2$ | 1.170 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0409, wR2 = 0.1039 | |
| R indices (all data) | R1 = 0.0537, wR2 = 0.1147 | |
| Extinction coefficient | 0 | |
| Largest diff. peak and hole | 0.821 and -0.596 e.$Å^{-3}$ | |

**Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$)**

U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Mn(1) | 6829(1) | 6773(1) | 10431(1) | 47(1) |
| I(1) | 8084(1) | 6827(1) | 10659(1) | 66(1) |
| C(1) | 6839(3) | 6712(3) | 11939(7) | 67(2) |
| O(1) | 6805(3) | 6678(3) | 12661(5) | 86(2) |
| C(2) | 6870(3) | 5910(3) | 10398(5) | 53(1) |
| O(2) | 6892(2) | 5387(2) | 10460(5) | 75(1) |
| C(3) | 5997(3) | 6758(3) | 10432(5) | 52(1) |
| O(3) | 5463(2) | 6747(2) | 10465(4) | 75(1) |
| C(4) | 6905(3) | 7636(3) | 10517(6) | 60(2) |
| O(4) | 6963(3) | 8159(2) | 10584(5) | 85(2) |
| C(5) | 6840(4) | 6845(4) | 8895(6) | 45(2) |
| O(5) | 7144(2) | 6540(2) | 8165(4) | 54(1) |
| C(6) | 6472(5) | 7301(4) | 8355(8) | 52(2) |
| S(1) | 6577(1) | 7397(1) | 7002(2) | 70(1) |
| C(7) | 6004(5) | 7710(5) | 8716(9) | 68(3) |
| C(8) | 5750(5) | 8051(6) | 7878(11) | 84(4) |
| C(9) | 6010(4) | 7940(4) | 6930(9) | 78(3) |
| C(10) | 7531(4) | 5994(3) | 8338(7) | 60(2) |
| C(11) | 7834(5) | 5855(5) | 7331(8) | 76(2) |
| C(5A) | 6810(20) | 6950(20) | 8783(13) | 42(9) |
| O(5A) | 6479(15) | 7313(14) | 8144(19) | 42(9) |
| C(6A) | 7208(17) | 6568(15) | 8129(11) | 73(4) |
| S(1A) | 7186(6) | 6652(6) | 6776(11) | 73(4) |
| C(7A) | 7640(20) | 6110(20) | 8391(19) | 73(4) |
| C(8A) | 7945(18) | 5841(17) | 7530(30) | 73(4) |
| C(9A) | 7741(10) | 6092(10) | 6610(20) | 73(4) |
| C(10A) | 6020(20) | 7761(19) | 8510(30) | 42(9) |
| C(11A) | 5753(19) | 8081(19) | 7580(40) | 42(9) |

**Table 3. Bond lengths [Å] and angles [°]**

| | | | |
|---|---|---|---|
| Mn(1)-C(3) | 1.784(6) | C(11A)-H(11D) | 0.96 |
| Mn(1)-C(2) | 1.851(6) | C(11A)-H(11E) | 0.96 |
| Mn(1)-C(4) | 1.862(6) | C(11A)-H(11F) | 0.96 |
| Mn(1)-C(1) | 1.949(10) | C(6A)-C(7A) | 1.390 |
| Mn(1)-C(5) | 1.986(8) | C(6A)-S(1A) | 1.755 |
| Mn(1)-C(5A) | 2.159(19) | S(1A)-C(9A) | 1.704 |
| Mn(1)-I(1) | 2.7090(13) | C(7A)-C(8A) | 1.409 |
| C(1)-O(1) | 0.937(9) | C(7A)-H(7A) | 0.93 |
| C(2)-O(2) | 1.126(7) | C(8A)-C(9A) | 1.378 |
| C(3)-O(3) | 1.145(7) | C(8A)-H(8A) | 0.93 |
| C(4)-O(4) | 1.131(7) | C(9A)-H(9A) | 0.93 |
| C(5)-O(5) | 1.318(8) | | |
| C(5)-C(6) | 1.437(9) | C(3)-Mn(1)-C(2) | 91.7(2) |
| O(5)-C(10) | 1.452(8) | C(3)-Mn(1)-C(4) | 96.0(3) |
| C(10)-C(11) | 1.482(11) | C(2)-Mn(1)-C(4) | 172.0(3) |
| C(10)-H(10A) | 0.97 | C(3)-Mn(1)-C(1) | 90.5(3) |
| C(10)-H(10B) | 0.97 | C(2)-Mn(1)-C(1) | 87.5(3) |
| C(11)-H(11A) | 0.96 | C(4)-Mn(1)-C(1) | 90.3(3) |
| C(11)-H(11B) | 0.96 | C(3)-Mn(1)-C(5) | 90.8(3) |
| C(11)-H(11C) | 0.96 | C(2)-Mn(1)-C(5) | 93.1(3) |
| C(6)-C(7) | 1.411(10) | C(4)-Mn(1)-C(5) | 88.9(3) |
| C(6)-S(1) | 1.770(11) | C(1)-Mn(1)-C(5) | 178.5(4) |
| S(1)-C(9) | 1.685(8) | C(3)-Mn(1)-C(5A) | 88.9(13) |
| C(7)-C(8) | 1.414(13) | C(2)-Mn(1)-C(5A) | 98.9(11) |
| C(7)-H(7) | 0.93 | C(4)-Mn(1)-C(5A) | 83.5(12) |
| C(8)-C(9) | 1.364(15) | C(1)-Mn(1)-C(5A) | 173.6(11) |
| C(8)-H(8) | 0.93 | C(5)-Mn(1)-C(5A) | 6.0(10) |
| C(9)-H(9) | 0.93 | C(3)-Mn(1)-I(1) | 173.5(2) |
| C(5A)-O(5A) | 1.333 | C(2)-Mn(1)-I(1) | 89.92(18) |
| C(5A)-C(6A) | 1.457 | C(4)-Mn(1)-I(1) | 82.19(19) |
| O(5A)-C(10A) | 1.450 | C(1)-Mn(1)-I(1) | 83.3(2) |
| C(10A)-C(11A) | 1.500 | C(5)-Mn(1)-I(1) | 95.4(3) |
| C(10A)-H(10C) | 0.97 | C(5A)-Mn(1)-I(1) | 97.0(13) |
| C(10A)-H(10D) | 0.97 | O(1)-C(1)-Mn(1) | 174.8(9) |

| | | | |
|---|---|---|---|
| O(2)-C(2)-Mn(1) | 174.6(6) | S(1)-C(9)-H(9) | 124.3 |
| O(3)-C(3)-Mn(1) | 177.9(6) | O(5A)-C(5A)-C(6A) | 106.2 |
| O(4)-C(4)-Mn(1) | 178.4(6) | O(5A)-C(5A)-Mn(1) | 136.4(14) |
| O(5)-C(5)-C(6) | 105.2(6) | C(6A)-C(5A)-Mn(1) | 117.2(14) |
| O(5)-C(5)-Mn(1) | 132.8(6) | C(5A)-O(5A)-C(10A) | 122.4 |
| C(6)-C(5)-Mn(1) | 122.0(6) | O(5A)-C(10A)-C(11A) | 107.3 |
| C(5)-O(5)-C(10) | 124.9(6) | O(5A)-C(10A)-H(10C) | 110.3 |
| O(5)-C(10)-C(11) | 106.2(7) | C(11A)-C(10A)-H(10C) | 110.3 |
| O(5)-C(10)-H(10A) | 110.5 | O(5A)-C(10A)-H(10D) | 110.3 |
| C(11)-C(10)-H(10A) | 110.5 | C(11A)-C(10A)-H(10D) | 110.3 |
| O(5)-C(10)-H(10B) | 110.5 | H(10C)-C(10A)-H(10D) | 108.5 |
| C(11)-C(10)-H(10B) | 110.5 | C(10A)-C(11A)-H(11D) | 109.5 |
| H(10A)-C(10)-H(10B) | 108.7 | C(10A)-C(11A)-H(11E) | 109.5 |
| C(10)-C(11)-H(11A) | 109.5 | H(11D)-C(11A)-H(11E) | 109.5 |
| C(10)-C(11)-H(11B) | 109.5 | C(10A)-C(11A)-H(11F) | 109.5 |
| H(11A)-C(11)-H(11B) | 109.5 | H(11D)-C(11A)-H(11F) | 109.5 |
| C(10)-C(11)-H(11C) | 109.5 | H(11E)-C(11A)-H(11F) | 109.5 |
| H(11A)-C(11)-H(11C) | 109.5 | C(7A)-C(6A)-C(5A) | 130.5 |
| H(11B)-C(11)-H(11C) | 109.5 | C(7A)-C(6A)-S(1A) | 109.4 |
| C(7)-C(6)-C(5) | 130.7(7) | C(5A)-C(6A)-S(1A) | 120.1 |
| C(7)-C(6)-S(1) | 110.1(6) | C(9A)-S(1A)-C(6A) | 91.9 |
| C(5)-C(6)-S(1) | 119.2(6) | C(6A)-C(7A)-C(8A) | 114.1 |
| C(9)-S(1)-C(6) | 92.5(5) | C(6A)-C(7A)-H(7A) | 123.0 |
| C(6)-C(7)-C(8) | 110.0(9) | C(8A)-C(7A)-H(7A) | 123.0 |
| C(6)-C(7)-H(7) | 125.0 | C(9A)-C(8A)-C(7A) | 111.8 |
| C(8)-C(7)-H(7) | 125.0 | C(9A)-C(8A)-H(8A) | 124.1 |
| C(9)-C(8)-C(7) | 116.0(9) | C(7A)-C(8A)-H(8A) | 124.1 |
| C(9)-C(8)-H(8) | 122.0 | C(8A)-C(9A)-S(1A) | 112.8 |
| C(7)-C(8)-H(8) | 122.0 | C(8A)-C(9A)-H(9A) | 123.6 |
| C(8)-C(9)-S(1) | 111.4(7) | S(1A)-C(9A)-H(9A) | 123.6 |
| C(8)-C(9)-H(9) | 124.3 | | |

**Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$).**

The anisotropic displacement factor exponent takes the form: $-2\pi^2[ h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12} ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Mn(1) | 45(1) | 40(1) | 57(1) | -2(1) | 1(1) | 1(1) |
| I(1) | 50(1) | 65(1) | 83(1) | 0(1) | -8(1) | -3(1) |
| C(1) | 67(4) | 46(3) | 86(5) | -5(4) | 30(4) | 6(3) |
| O(1) | 98(4) | 83(4) | 76(4) | -17(3) | -19(4) | 11(3) |
| C(2) | 47(3) | 48(3) | 65(4) | 2(3) | 2(3) | 4(2) |
| O(2) | 78(3) | 44(2) | 104(4) | 8(2) | 8(3) | 0(2) |
| C(3) | 53(3) | 45(3) | 59(3) | -1(3) | 9(3) | 1(2) |
| O(3) | 45(2) | 79(3) | 101(4) | 5(3) | 12(2) | -4(2) |
| C(4) | 54(3) | 55(4) | 71(4) | -2(3) | -1(3) | 4(3) |
| O(4) | 96(4) | 47(3) | 112(5) | -11(3) | -1(3) | 2(2) |
| C(5) | 46(4) | 31(3) | 58(4) | -1(3) | -2(3) | -5(3) |
| O(5) | 58(3) | 46(2) | 58(3) | -3(2) | 2(2) | 1(2) |
| C(6) | 53(4) | 48(4) | 54(5) | 9(4) | -4(4) | -2(3) |
| S(1) | 73(1) | 70(1) | 67(1) | 9(1) | -12(1) | 1(1) |
| C(7) | 64(5) | 55(4) | 83(7) | 20(5) | -10(5) | 7(4) |
| C(8) | 68(6) | 81(6) | 103(10) | 27(6) | -10(6) | 14(4) |
| C(9) | 64(5) | 73(5) | 98(7) | 20(5) | -25(5) | 8(4) |
| C(10) | 61(5) | 48(4) | 72(5) | -11(3) | -4(4) | 13(4) |
| C(11) | 74(5) | 72(5) | 80(6) | -24(5) | 14(5) | 2(4) |

**Table 5. Hydrogen coordinates ( $x 10^4$) and isotropic displacement parameters ($Å^2 x 10^3$).**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(7) | 5881 | 7750 | 9405 | 81 |
| H(8) | 5426 | 8334 | 7967 | 101 |
| H(9) | 5890 | 8139 | 6321 | 94 |
| H(10A) | 7277 | 5643 | 8561 | 72 |
| H(10B) | 7842 | 6077 | 8866 | 72 |

| | | | | |
|---|---|---|---|---|
| H(11A) | 8099 | 5496 | 7405 | 114 |
| H(11B) | 8081 | 6207 | 7119 | 114 |
| H(11C) | 7521 | 5772 | 6818 | 114 |
| H(7A) | 7724 | 5997 | 9073 | 88 |
| H(8A) | 8246 | 5531 | 7585 | 88 |
| H(9A) | 7890 | 5968 | 5965 | 88 |
| H(10C) | 6223 | 8064 | 8965 | 50 |
| H(10D) | 5698 | 7551 | 8901 | 50 |
| H(11D) | 5449 | 8383 | 7794 | 63 |
| H(11E) | 5558 | 7778 | 7136 | 63 |
| H(11F) | 6080 | 8288 | 7200 | 63 |

**Table 6. Torsion angles [°].**

| | | | |
|---|---|---|---|
| C(3)-Mn(1)-C(5)-O(5) | -130.6(7) | C(5)-O(5)-C(10)-C(11) | -173.7(7) |
| C(2)-Mn(1)-C(5)-O(5) | -38.9(7) | O(5)-C(5)-C(6)-C(7) | 172.0(8) |
| C(4)-Mn(1)-C(5)-O(5) | 133.4(7) | Mn(1)-C(5)-C(6)-C(7) | -8.6(11) |
| C(5A)-Mn(1)-C(5)-O(5) | 158(17) | O(5)-C(5)-C(6)-S(1) | -6.8(8) |
| I(1)-Mn(1)-C(5)-O(5) | 51.4(7) | Mn(1)-C(5)-C(6)-S(1) | 172.6(6) |
| C(3)-Mn(1)-C(5)-C(6) | 50.1(6) | C(7)-C(6)-S(1)-C(9) | -1.4(6) |
| C(2)-Mn(1)-C(5)-C(6) | 141.9(6) | C(5)-C(6)-S(1)-C(9) | 177.6(7) |
| C(4)-Mn(1)-C(5)-C(6) | -45.8(6) | C(5)-C(6)-C(7)-C(8) | -176.7(8) |
| C(5A)-Mn(1)-C(5)-C(6) | -22(16) | S(1)-C(6)-C(7)-C(8) | 2.2(9) |
| I(1)-Mn(1)-C(5)-C(6) | -127.9(5) | C(6)-C(7)-C(8)-C(9) | -2.2(13) |
| C(6)-C(5)-O(5)-C(10) | -173.8(6) | C(7)-C(8)-C(9)-S(1) | 1.1(13) |
| Mn(1)-C(5)-O(5)-C(10) | 6.8(11) | C(6)-S(1)-C(9)-C(8) | 0.2(8) |

# Appendix 5

## Crystallographic data of Complex 8

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

| | | |
|---|---|---|
| Identification code | dbamco2 | |
| Empirical formula | $C_{14}$ $H_5$ $Mn_2$ N $O_9$ S | |
| Formula weight | 473.13 | |
| Temperature | 293(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P $2_1$/n | |
| Unit cell dimensions | a = 14.4298(8) Å | α = 90°. |
| | b = 9.1653(5) Å | β = 113.7790(10)°. |
| | c = 14.7785(8) Å | γ = 90°. |
| Volume | 1788.58(17) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.757 $Mg/m^3$ | |
| Absorption coefficient | 1.576 $mm^{-1}$ | |
| F(000) | 936 | |
| Crystal size | 0.32 x 0.28 x 0.20 $mm^3$ | |
| Theta range for data collection | 2.68 to 26.54°. | |
| Index ranges | -13<=h<=17, -11<=k<=11, -14<=l<=17 | |
| Reflections collected | 9351 | |
| Independent reflections | 3345 [R(int) = 0.0260] | |
| Completeness to theta = 25.00° | 99.2 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.730 and 0.549 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3345 / 0 / 256 | |
| Goodness-of-fit on $F^2$ | 1.060 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0397, wR2 = 0.1198 | |
| R indices (all data) | R1 = 0.0440, wR2 = 0.1263 | |
| Extinction coefficient | 0 | |
| Largest diff. peak and hole | 0.840 and -0.806 $e.Å^{-3}$ | |

**Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$)**

U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Mn(1) | 7960(1) | 9395(1) | -328(1) | 47(1) |
| Mn(2) | 7392(1) | 6434(1) | -8(1) | 37(1) |
| C(1) | 8320(3) | 11250(4) | -483(3) | 67(1) |
| O(1) | 8545(3) | 12403(3) | -581(3) | 99(1) |
| C(2) | 9077(3) | 9072(4) | 823(3) | 59(1) |
| O(2) | 9783(2) | 8890(4) | 1528(2) | 82(1) |
| C(3) | 7223(3) | 9914(4) | 392(2) | 54(1) |
| O(3) | 6775(2) | 10274(3) | 838(2) | 74(1) |
| C(4) | 6799(3) | 9452(4) | -1477(3) | 62(1) |
| O(4) | 6074(3) | 9498(4) | -2178(2) | 100(1) |
| C(5) | 8637(3) | 8528(4) | -1015(3) | 59(1) |
| O(5) | 9067(3) | 8013(4) | -1424(3) | 88(1) |
| C(6) | 7007(2) | 4602(3) | 83(2) | 47(1) |
| O(6) | 6757(2) | 3422(3) | 115(2) | 70(1) |
| C(7) | 6107(2) | 7221(3) | -475(2) | 47(1) |
| O(7) | 5296(2) | 7661(3) | -827(2) | 70(1) |
| C(8) | 7214(2) | 6103(4) | -1293(2) | 52(1) |
| O(8) | 7102(2) | 5825(4) | -2081(2) | 83(1) |
| C(9) | 8738(2) | 5934(4) | 398(2) | 49(1) |
| O(9) | 9558(2) | 5581(3) | 657(2) | 73(1) |
| C(10) | 7620(2) | 6780(3) | 1415(2) | 40(1) |
| N(1) | 8506(2) | 6826(4) | 2170(2) | 59(1) |
| S(1) | 5742(1) | 5918(2) | 1319(1) | 81(1) |
| C(11) | 6810(2) | 6932(3) | 1766(2) | 42(1) |
| C(12) | 6818(2) | 7950(3) | 2560(2) | 45(1) |
| C(13) | 5887(4) | 7684(6) | 2661(3) | 77(1) |
| C(14) | 5278(3) | 6691(6) | 2069(3) | 78(1) |

**Table 3. Bond lengths [Å] and angles [°]**

| | | | |
|---|---|---|---|
| Mn(1)-C(1) | 1.820(4) | Mn(1)-C(4) | 1.843(4) |
| Mn(1)-C(2) | 1.836(4) | Mn(1)-C(3) | 1.845(3) |

| | | | |
|---|---|---|---|
| Mn(1)-C(5) | 1.849(4) | C(2)-Mn(1)-C(4) | 172.15(16) |
| Mn(1)-Mn(2) | 2.9280(6) | C(1)-Mn(1)-C(3) | 95.26(16) |
| Mn(2)-C(6) | 1.790(3) | C(2)-Mn(1)-C(3) | 90.08(16) |
| Mn(2)-C(8) | 1.836(3) | C(4)-Mn(1)-C(3) | 90.20(16) |
| Mn(2)-C(7) | 1.845(3) | C(1)-Mn(1)-C(5) | 95.24(16) |
| Mn(2)-C(9) | 1.845(3) | C(2)-Mn(1)-C(5) | 88.77(17) |
| Mn(2)-C(10) | 2.019(3) | C(4)-Mn(1)-C(5) | 89.52(17) |
| C(1)-O(1) | 1.132(5) | C(3)-Mn(1)-C(5) | 169.49(15) |
| C(2)-O(2) | 1.138(5) | C(1)-Mn(1)-Mn(2) | 177.99(13) |
| C(3)-O(3) | 1.141(4) | C(2)-Mn(1)-Mn(2) | 84.21(11) |
| C(4)-O(4) | 1.138(5) | C(4)-Mn(1)-Mn(2) | 88.03(12) |
| C(5)-O(5) | 1.128(4) | C(3)-Mn(1)-Mn(2) | 83.22(10) |
| C(6)-O(6) | 1.147(4) | C(5)-Mn(1)-Mn(2) | 86.27(11) |
| C(7)-O(7) | 1.145(4) | C(6)-Mn(2)-C(8) | 90.28(15) |
| C(8)-O(8) | 1.137(4) | C(6)-Mn(2)-C(7) | 95.70(13) |
| C(9)-O(9) | 1.133(4) | C(8)-Mn(2)-C(7) | 88.73(14) |
| C(10)-N(1) | 1.315(4) | C(6)-Mn(2)-C(9) | 93.48(14) |
| C(10)-C(11) | 1.464(4) | C(8)-Mn(2)-C(9) | 89.14(14) |
| N(1)-H(1A) | 0.77(5) | C(7)-Mn(2)-C(9) | 170.58(14) |
| N(1)-H(1B) | 0.85(5) | C(6)-Mn(2)-C(10) | 89.69(13) |
| S(1)-C(14) | 1.667(5) | C(8)-Mn(2)-C(10) | 178.68(13) |
| S(1)-C(11) | 1.690(3) | C(7)-Mn(2)-C(10) | 92.59(12) |
| C(11)-C(12) | 1.496(4) | C(9)-Mn(2)-C(10) | 89.55(12) |
| C(12)-C(13) | 1.431(5) | C(6)-Mn(2)-Mn(1) | 175.42(10) |
| C(12)-H(12) | 0.93(5) | C(8)-Mn(2)-Mn(1) | 85.25(11) |
| C(13)-C(14) | 1.321(7) | C(7)-Mn(2)-Mn(1) | 83.20(9) |
| C(13)-H(13) | 0.84(5) | C(9)-Mn(2)-Mn(1) | 87.48(10) |
| C(14)-H(14) | 0.94(5) | C(10)-Mn(2)-Mn(1) | 94.80(8) |
| C(1)-Mn(1)-C(2) | 94.48(18) | O(1)-C(1)-Mn(1) | 179.8(4) |
| C(1)-Mn(1)-C(4) | 93.31(19) | O(2)-C(2)-Mn(1) | 178.3(3) |

| | | | |
|---|---|---|---|
| O(3)-C(3)-Mn(1) | 178.1(3) | C(14)-S(1)-C(11) | 93.09(19) |
| O(4)-C(4)-Mn(1) | 178.8(4) | C(10)-C(11)-C(12) | 125.6(2) |
| O(5)-C(5)-Mn(1) | 178.7(4) | C(10)-C(11)-S(1) | 122.8(2) |
| O(6)-C(6)-Mn(2) | 178.1(3) | C(12)-C(11)-S(1) | 111.5(2) |
| O(7)-C(7)-Mn(2) | 175.1(3) | C(13)-C(12)-C(11) | 105.4(3) |
| O(8)-C(8)-Mn(2) | 176.5(3) | C(13)-C(12)-H(12) | 127(3) |
| O(9)-C(9)-Mn(2) | 177.6(3) | C(11)-C(12)-H(12) | 127(3) |
| N(1)-C(10)-C(11) | 109.8(3) | C(14)-C(13)-C(12) | 116.8(4) |
| N(1)-C(10)-Mn(2) | 125.7(2) | C(14)-C(13)-H(13) | 130(4) |
| C(11)-C(10)-Mn(2) | 124.43(19) | C(12)-C(13)-H(13) | 112(4) |
| C(10)-N(1)-H(1A) | 124(4) | C(13)-C(14)-S(1) | 113.2(3) |
| C(10)-N(1)-H(1B) | 124(3) | C(13)-C(14)-H(14) | 121(3) |
| H(1A)-N(1)-H(1B) | 111(5) | S(1)-C(14)-H(14) | 126(3) |

**Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)**

The anisotropic displacement factor exponent takes the form: $-2\pi^2[ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12} ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Mn(1) | 53(1) | 44(1) | 51(1) | 2(1) | 29(1) | -3(1) |
| Mn(2) | 37(1) | 40(1) | 34(1) | -2(1) | 13(1) | -2(1) |
| C(1) | 78(2) | 56(2) | 87(3) | 3(2) | 52(2) | -4(2) |
| O(1) | 127(3) | 50(2) | 157(3) | 5(2) | 94(3) | -16(2) |
| C(2) | 55(2) | 57(2) | 65(2) | -6(2) | 26(2) | -12(2) |
| O(2) | 66(2) | 87(2) | 77(2) | -5(2) | 13(2) | -15(2) |
| C(3) | 64(2) | 45(2) | 58(2) | 1(1) | 32(2) | -6(1) |
| O(3) | 103(2) | 56(1) | 92(2) | -3(1) | 69(2) | 0(1) |
| C(4) | 69(2) | 67(2) | 57(2) | 13(2) | 30(2) | 5(2) |
| O(4) | 91(2) | 126(3) | 64(2) | 26(2) | 13(2) | 13(2) |
| C(5) | 64(2) | 60(2) | 65(2) | 6(2) | 37(2) | -4(2) |
| O(5) | 104(2) | 89(2) | 106(2) | 0(2) | 79(2) | 4(2) |
| C(6) | 44(2) | 47(2) | 45(2) | -2(1) | 11(1) | 0(1) |
| O(6) | 75(2) | 41(1) | 87(2) | 2(1) | 26(1) | -8(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(7) | 48(2) | 49(2) | 40(1) | 1(1) | 14(1) | -4(1) |
| O(7) | 41(1) | 80(2) | 75(2) | 15(1) | 9(1) | 7(1) |
| C(8) | 52(2) | 58(2) | 46(2) | -7(1) | 19(1) | -3(1) |
| O(8) | 94(2) | 112(2) | 46(1) | -22(1) | 33(1) | -7(2) |
| C(9) | 46(2) | 53(2) | 47(2) | -4(1) | 19(1) | 1(1) |
| O(9) | 52(1) | 90(2) | 76(2) | -4(1) | 25(1) | 14(1) |
| C(10) | 41(1) | 40(1) | 37(1) | 2(1) | 13(1) | -6(1) |
| N(1) | 43(1) | 88(2) | 39(1) | 2(1) | 11(1) | -11(1) |
| S(1) | 63(1) | 113(1) | 75(1) | -29(1) | 38(1) | -28(1) |
| C(11) | 47(1) | 43(1) | 36(1) | 1(1) | 16(1) | -4(1) |
| C(12) | 57(2) | 47(2) | 41(1) | -3(1) | 30(1) | -7(1) |
| C(13) | 93(3) | 90(3) | 63(2) | -8(2) | 47(2) | 7(2) |
| C(14) | 60(2) | 116(4) | 67(2) | -2(2) | 35(2) | -6(2) |

**Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$x $10^3$)**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 9020(40) | 6930(60) | 2120(40) | 88 |
| H(1B) | 8580(40) | 6900(60) | 2770(40) | 88 |
| H(12) | 7320(40) | 8610(60) | 2910(40) | 54 |
| H(13) | 5870(40) | 8110(60) | 3160(40) | 92 |
| H(14) | 4650(40) | 6460(50) | 2100(40) | 94 |

**Table 6. Torsion angles [°]**

| | | | |
|---|---|---|---|
| C(2)-Mn(1)-Mn(2)-C(8) | -129.31(15) | C(5)-Mn(1)-Mn(2)-C(7) | -129.45(15) |
| C(4)-Mn(1)-Mn(2)-C(8) | 49.48(16) | C(2)-Mn(1)-Mn(2)-C(9) | -39.96(15) |
| C(3)-Mn(1)-Mn(2)-C(8) | 139.92(15) | C(4)-Mn(1)-Mn(2)-C(9) | 138.83(15) |
| C(5)-Mn(1)-Mn(2)-C(8) | -40.16(16) | C(3)-Mn(1)-Mn(2)-C(9) | -130.74(15) |
| C(2)-Mn(1)-Mn(2)-C(7) | 141.41(15) | C(5)-Mn(1)-Mn(2)-C(9) | 49.18(15) |
| C(4)-Mn(1)-Mn(2)-C(7) | -39.80(15) | C(2)-Mn(1)-Mn(2)-C(10) | 49.37(14) |
| C(3)-Mn(1)-Mn(2)-C(7) | 50.64(14) | C(4)-Mn(1)-Mn(2)-C(10) | -131.84(14) |

| | | | |
|---|---|---|---|
| C(3)-Mn(1)-Mn(2)-C(10) | -41.40(14) | | |
| C(5)-Mn(1)-Mn(2)-C(10) | 138.51(14) | Mn(2)-C(10)-C(11)-C(12) | -142.7(2) |
| C(6)-Mn(2)-C(10)-N(1) | 103.9(3) | N(1)-C(10)-C(11)-S(1) | -137.9(3) |
| C(7)-Mn(2)-C(10)-N(1) | -160.4(3) | Mn(2)-C(10)-C(11)-S(1) | 38.8(3) |
| C(9)-Mn(2)-C(10)-N(1) | 10.4(3) | C(14)-S(1)-C(11)-C(10) | 178.9(3) |
| Mn(1)-Mn(2)-C(10)-N(1) | -77.1(3) | C(14)-S(1)-C(11)-C(12) | 0.2(3) |
| C(6)-Mn(2)-C(10)-C(11) | -72.3(3) | C(10)-C(11)-C(12)-C(13) | -178.5(3) |
| C(7)-Mn(2)-C(10)-C(11) | 23.4(3) | S(1)-C(11)-C(12)-C(13) | 0.2(3) |
| C(9)-Mn(2)-C(10)-C(11) | -165.8(3) | C(11)-C(12)-C(13)-C(14) | -0.6(5) |
| Mn(1)-Mn(2)-C(10)-C(11) | 106.7(2) | C(12)-C(13)-C(14)-S(1) | 0.8(6) |
| N(1)-C(10)-C(11)-C(12) | 40.6(4) | C(11)-S(1)-C(14)-C(13) | -0.6(4) |

# Appendix 6

## Crystallographic data of Complex 9

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

| | | |
|---|---|---|
| Identification code | dbamco3a_abs | |
| Empirical formula | $C_{14}$ $H_5$ $Mn_2$ N $O_{10}$ | |
| Formula weight | 457.07 | |
| Temperature | 293(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/c | |
| Unit cell dimensions | a = 12.0713(9) Å | α = 90º. |
| | b = 9.0817(7) Å | β = 92.5930(10)º. |
| | c = 15.8406(12) Å | γ = 90º. |
| Volume | 1734.8(2) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.750 $Mg/m^3$ | |
| Absorption coefficient | 1.510 $mm^{-1}$ | |
| F(000) | 904 | |
| Crystal size | 0.36 x 0.34 x 0.24 $mm^3$ | |
| Theta range for data collection | 2.57 to 26.49º. | |
| Index ranges | -14<=h<=11, -11<=k<=5, -19<=l<=19 | |
| Reflections collected | 9176 | |
| Independent reflections | 3301 [R(int) = 0.0224] | |
| Completeness to theta = 25.00º | 99.8 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.696 and 0.587 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3301 / 0 / 265 | |
| Goodness-of-fit on $F^2$ | 1.091 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0274, wR2 = 0.0727 | |
| R indices (all data) | R1 = 0.0299, wR2 = 0.0760 | |
| Extinction coefficient | 0.0014(5) | |
| Largest diff. peak and hole | 0.258 and -0.233 $e.Å^{-3}$ | |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Mn(1) | 8297(1) | 4141(1) | 8790(1) | 45(1) |
| Mn(2) | 7333(1) | 1182(1) | 8648(1) | 38(1) |
| C(1) | 8815(2) | 6012(2) | 8839(1) | 62(1) |
| O(1) | 9128(2) | 7193(2) | 8872(1) | 93(1) |
| C(2) | 8200(2) | 3952(2) | 9942(1) | 58(1) |
| O(2) | 8159(2) | 3873(2) | 10655(1) | 84(1) |
| C(3) | 6809(2) | 4644(2) | 8706(1) | 51(1) |
| O(3) | 5912(1) | 4986(2) | 8658(1) | 72(1) |
| C(4) | 8358(2) | 4048(2) | 7628(1) | 57(1) |
| O(4) | 8412(2) | 4009(2) | 6917(1) | 86(1) |
| C(5) | 9672(2) | 3255(2) | 8875(1) | 61(1) |
| O(5) | 10524(1) | 2737(2) | 8928(1) | 92(1) |
| C(6) | 6749(2) | -622(2) | 8512(1) | 53(1) |
| O(6) | 6374(2) | -1763(2) | 8415(1) | 84(1) |
| C(7) | 6594(1) | 1934(2) | 7706(1) | 49(1) |
| O(7) | 6189(1) | 2349(2) | 7085(1) | 75(1) |
| C(8) | 8478(2) | 730(2) | 7970(1) | 54(1) |
| O(8) | 9165(1) | 389(2) | 7546(1) | 86(1) |
| C(9) | 8256(2) | 682(2) | 9569(1) | 49(1) |
| O(9) | 8826(1) | 328(2) | 10120(1) | 73(1) |
| C(10) | 6100(1) | 1643(2) | 9435(1) | 41(1) |
| N(1) | 6227(2) | 1718(2) | 10260(1) | 60(1) |
| O(10) | 4243(1) | 2348(2) | 9753(1) | 71(1) |
| C(11) | 4946(1) | 1838(2) | 9159(1) | 45(1) |
| C(12) | 4340(2) | 1582(3) | 8442(1) | 62(1) |
| C(13) | 3232(2) | 1979(3) | 8585(2) | 77(1) |
| C(14) | 3213(2) | 2416(3) | 9368(2) | 81(1) |

**Table 3. Bond lengths [Å] and angles [º]**

| | | | |
|---|---|---|---|
| Mn(1)-C(1) | 1.8106(19) | C(1)-Mn(1)-C(5) | 95.61(9) |
| Mn(1)-C(2) | 1.841(2) | C(2)-Mn(1)-C(5) | 89.12(9) |
| Mn(1)-C(5) | 1.844(2) | C(1)-Mn(1)-C(4) | 93.19(9) |
| Mn(1)-C(4) | 1.849(2) | C(2)-Mn(1)-C(4) | 171.91(9) |
| Mn(1)-C(3) | 1.8518(19) | C(5)-Mn(1)-C(4) | 88.60(9) |
| Mn(1)-Mn(2) | 2.9331(4) | C(1)-Mn(1)-C(3) | 95.98(9) |
| Mn(2)-C(6) | 1.7928(19) | C(2)-Mn(1)-C(3) | 89.43(9) |
| Mn(2)-C(8) | 1.8355(19) | C(5)-Mn(1)-C(3) | 168.40(8) |
| Mn(2)-C(7) | 1.8364(17) | C(4)-Mn(1)-C(3) | 91.25(9) |
| Mn(2)-C(9) | 1.8506(18) | C(1)-Mn(1)-Mn(2) | 176.33(7) |
| Mn(2)-C(10) | 2.0275(16) | C(2)-Mn(1)-Mn(2) | 87.01(6) |
| C(1)-O(1) | 1.138(2) | C(5)-Mn(1)-Mn(2) | 87.62(6) |
| C(2)-O(2) | 1.135(2) | C(4)-Mn(1)-Mn(2) | 85.14(6) |
| C(3)-O(3) | 1.126(2) | C(3)-Mn(1)-Mn(2) | 80.81(5) |
| C(4)-O(4) | 1.131(2) | C(6)-Mn(2)-C(8) | 91.59(9) |
| C(5)-O(5) | 1.131(2) | C(6)-Mn(2)-C(7) | 93.94(8) |
| C(6)-O(6) | 1.138(2) | C(8)-Mn(2)-C(7) | 87.61(8) |
| C(7)-O(7) | 1.141(2) | C(6)-Mn(2)-C(9) | 95.15(8) |
| C(8)-O(8) | 1.133(2) | C(8)-Mn(2)-C(9) | 87.92(8) |
| C(9)-O(9) | 1.134(2) | C(7)-Mn(2)-C(9) | 169.98(8) |
| C(10)-N(1) | 1.310(2) | C(6)-Mn(2)-C(10) | 88.10(8) |
| C(10)-C(11) | 1.452(2) | C(8)-Mn(2)-C(10) | 177.79(7) |
| N(1)-H(1A) | 0.90(2) | C(7)-Mn(2)-C(10) | 94.60(7) |
| N(1)-H(1B) | 0.77(2) | C(9)-Mn(2)-C(10) | 89.92(7) |
| O(10)-C(14) | 1.361(3) | C(6)-Mn(2)-Mn(1) | 177.51(6) |
| O(10)-C(11) | 1.376(2) | C(8)-Mn(2)-Mn(1) | 86.75(6) |
| C(11)-C(12) | 1.344(3) | C(7)-Mn(2)-Mn(1) | 84.14(6) |
| C(12)-C(13) | 1.414(3) | C(9)-Mn(2)-Mn(1) | 86.66(6) |
| C(12)-H(12) | 0.87(2) | C(10)-Mn(2)-Mn(1) | 93.63(4) |
| C(13)-C(14) | 1.304(4) | O(1)-C(1)-Mn(1) | 179.1(2) |
| C(13)-H(13) | 0.85(3) | O(2)-C(2)-Mn(1) | 177.92(19) |
| C(14)-H(14) | 0.95(3) | O(3)-C(3)-Mn(1) | 178.20(17) |
| | | O(4)-C(4)-Mn(1) | 178.7(2) |
| C(1)-Mn(1)-C(2) | 94.75(9) | O(5)-C(5)-Mn(1) | 178.8(2) |

| | | | |
|---|---|---|---|
| O(6)-C(6)-Mn(2) | 179.03(19) | C(12)-C(11)-C(10) | 135.38(16) |
| O(7)-C(7)-Mn(2) | 175.00(16) | O(10)-C(11)-C(10) | 116.64(15) |
| O(8)-C(8)-Mn(2) | 176.9(2) | C(11)-C(12)-C(13) | 107.7(2) |
| O(9)-C(9)-Mn(2) | 177.56(17) | C(11)-C(12)-H(12) | 128.0(16) |
| N(1)-C(10)-C(11) | 111.20(15) | C(13)-C(12)-H(12) | 124.3(16) |
| N(1)-C(10)-Mn(2) | 124.59(14) | C(14)-C(13)-C(12) | 106.7(2) |
| C(11)-C(10)-Mn(2) | 124.10(11) | C(14)-C(13)-H(13) | 129(2) |
| C(10)-N(1)-H(1A) | 121.2(13) | C(12)-C(13)-H(13) | 124(2) |
| C(10)-N(1)-H(1B) | 124.3(17) | C(13)-C(14)-O(10) | 111.0(2) |
| H(1A)-N(1)-H(1B) | 114(2) | C(13)-C(14)-H(14) | 135.2(18) |
| C(14)-O(10)-C(11) | 106.72(17) | O(10)-C(14)-H(14) | 113.7(18) |
| C(12)-C(11)-O(10) | 107.91(16) | | |

**Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)**

The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Mn(1) | 42(1) | 42(1) | 50(1) | 4(1) | 3(1) | -3(1) |
| Mn(2) | 41(1) | 39(1) | 34(1) | 0(1) | 5(1) | 0(1) |
| C(1) | 56(1) | 52(1) | 76(1) | 3(1) | 5(1) | -5(1) |
| O(1) | 93(1) | 52(1) | 133(2) | 0(1) | 9(1) | -22(1) |
| C(2) | 62(1) | 52(1) | 58(1) | 1(1) | 0(1) | -6(1) |
| O(2) | 110(1) | 92(1) | 50(1) | -1(1) | -2(1) | -16(1) |
| C(3) | 51(1) | 42(1) | 59(1) | 5(1) | 5(1) | 0(1) |
| O(3) | 51(1) | 58(1) | 108(1) | 9(1) | 5(1) | 7(1) |
| C(4) | 58(1) | 56(1) | 59(1) | 11(1) | 10(1) | -2(1) |
| O(4) | 106(1) | 98(1) | 56(1) | 12(1) | 19(1) | -10(1) |
| C(5) | 51(1) | 59(1) | 72(1) | 9(1) | 2(1) | -5(1) |
| O(5) | 48(1) | 97(1) | 132(2) | 21(1) | 3(1) | 12(1) |
| C(6) | 64(1) | 51(1) | 44(1) | -3(1) | 5(1) | -3(1) |
| O(6) | 118(1) | 53(1) | 81(1) | -9(1) | 0(1) | -28(1) |
| C(7) | 46(1) | 62(1) | 39(1) | 2(1) | 8(1) | -3(1) |
| O(7) | 67(1) | 114(1) | 43(1) | 21(1) | -6(1) | -6(1) |
| C(8) | 56(1) | 56(1) | 52(1) | 3(1) | 8(1) | 9(1) |
| O(8) | 75(1) | 104(1) | 81(1) | -5(1) | 35(1) | 25(1) |
| C(9) | 50(1) | 49(1) | 49(1) | 3(1) | 4(1) | 5(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O(9) | 69(1) | 89(1) | 60(1) | 11(1) | -11(1) | 18(1) |
| C(10) | 48(1) | 40(1) | 36(1) | 1(1) | 7(1) | -7(1) |
| N(1) | 53(1) | 90(1) | 36(1) | -4(1) | 6(1) | -8(1) |
| O(10) | 56(1) | 96(1) | 63(1) | -17(1) | 16(1) | 9(1) |
| C(11) | 45(1) | 47(1) | 44(1) | 0(1) | 12(1) | -4(1) |
| C(12) | 50(1) | 85(1) | 51(1) | -6(1) | 6(1) | -9(1) |
| C(13) | 46(1) | 101(2) | 83(2) | 9(1) | -1(1) | -4(1) |
| C(14) | 50(1) | 99(2) | 96(2) | -5(1) | 18(1) | 14(1) |

**Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$x $10^3$)**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 5654(19) | 1920(20) | 10580(14) | 62(6) |
| H(1B) | 6785(19) | 1600(30) | 10510(14) | 60(7) |
| H(12) | 4560(20) | 1220(30) | 7968(15) | 74(7) |
| H(13) | 2710(20) | 1980(30) | 8206(18) | 97(9) |
| H(14) | 2660(20) | 2800(30) | 9717(18) | 103(9) |

**Table 6. Torsion angles [º]**

| | | | |
|---|---|---|---|
| C2)-Mn(1)-Mn(2)-C(8) | -129.88(9) | C(3)-Mn(1)-Mn(2)-C(10) | -41.97(7) |
| C(5)-Mn(1)-Mn(2)-C(8) | -40.64(9) | C(6)-Mn(2)-C(10)-N(1) | 105.07(16) |
| C(4)-Mn(1)-Mn(2)-C(8) | 48.15(9) | C(7)-Mn(2)-C(10)-N(1) | -161.13(16) |
| C(3)-Mn(1)-Mn(2)-C(8) | 140.21(8) | C(9)-Mn(2)-C(10)-N(1) | 9.92(16) |
| C(2)-Mn(1)-Mn(2)-C(7) | 142.19(8) | Mn(1)-Mn(2)-C(10)-N(1) | -76.73(15) |
| C(5)-Mn(1)-Mn(2)-C(7) | -128.57(9) | C(6)-Mn(2)-C(10)-C(11) | -70.79(14) |
| C(4)-Mn(1)-Mn(2)-C(7) | -39.77(8) | C(7)-Mn(2)-C(10)-C(11) | 23.00(14) |
| C(3)-Mn(1)-Mn(2)-C(7) | 52.29(8) | C(9)-Mn(2)-C(10)-C(11) | -165.95(14) |
| C(2)-Mn(1)-Mn(2)-C(9) | -41.77(9) | Mn(1)-Mn(2)-C(10)-C(11) | 107.41(13) |
| C(5)-Mn(1)-Mn(2)-C(9) | 47.46(9) | C(14)-O(10)-C(11)-C(12) | -1.2(2) |
| C(4)-Mn(1)-Mn(2)-C(9) | 136.26(9) | C(14)-O(10)-C(11)-C(10) | -178.64(18) |
| C(3)-Mn(1)-Mn(2)-C(9) | -131.68(8) | N(1)-C(10)-C(11)-C(12) | -164.1(2) |
| C(2)-Mn(1)-Mn(2)-C(10) | 47.93(8) | Mn(2)-C(10)-C(11)-C(12) | 12.3(3) |
| C(5)-Mn(1)-Mn(2)-C(10) | 137.17(8) | N(1)-C(10)-C(11)-O(10) | 12.5(2) |
| C(4)-Mn(1)-Mn(2)-C(10) | -134.03(8) | Mn(2)-C(10)-C(11)-O(10) | -171.13(12) |

| | | | |
|---|---|---|---|
| O(10)-C(11)-C(12)-C(13) | 1.5(2) | C(12)-C(13)-C(14)-O(10) | 0.6(3) |
| C(10)-C(11)-C(12)-C(13) | 178.3(2) | C(11)-O(10)-C(14)-C(13) | 0.3(3) |
| C(11)-C(12)-C(13)-C(14) | -1.3(3) | | |

# Appendix 7

## Crystallographic data of Complex 11

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

| | | |
|---|---|---|
| Identification code | dbamc08al_abs3 | |
| Empirical formula | $C_{17}H_{11}Mn_2NO_{10}$ | |
| Formula weight | 499.15 | |
| Temperature | 293(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | monoclinic | |
| Space group | $P2_1/c$ | |
| Unit cell dimensions | a = 12.7412(13) Å | α = 90º. |
| | b = 12.9836(13) Å | β = 90.0000(10)º. |
| | c = 12.6967(12) Å | γ = 90º. |
| Volume | 2100.4(4) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.578 $Mg/m^3$ | |
| Absorption coefficient | 1.254 $mm^{-1}$ | |
| F(000) | 1000 | |
| Crystal size | 0.46 x 0.24 x 0.16 $mm^3$ | |
| Theta range for data collection | 2.76 to 26.44º. | |
| Index ranges | -15<=h<=15, -15<=k<=16, -15<=l<=5 | |
| Reflections collected | 10635 | |
| Independent reflections | 3943 [R(int) = 0.0272] | |
| Completeness to theta = 25.00º | 99.5 % | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3943 / 0 / 311 | |
| Goodness-of-fit on $F^2$ | 1.073 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0522, wR2 = 0.1418 | |
| R indices (all data) | R1 = 0.0703, wR2 = 0.1592 | |
| Largest diff. peak and hole | 0.505 and -0.337 $e.Å^{-3}$ | |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Mn(1) | 1194(1) | 1515(1) | 8294(1) | 68(1) |
| Mn(2) | 2875(1) | 347(1) | 7287(1) | 67(1) |
| C(1) | 198(4) | 2246(5) | 8962(4) | 94(2) |
| O(1) | -421(3) | 2714(4) | 9406(4) | 131(2) |
| C(2) | 1244(4) | 2369(5) | 7135(4) | 91(2) |
| O(2) | 1261(4) | 2922(4) | 6436(3) | 132(2) |
| C(3) | 294(4) | 657(5) | 7557(4) | 94(2) |
| O(3) | -272(3) | 140(5) | 7116(4) | 139(2) |
| C(4) | 1266(3) | 539(4) | 9344(3) | 76(1) |
| O(4) | 1287(3) | -45(3) | 10008(3) | 104(1) |
| C(5) | 2278(4) | 2237(4) | 8903(3) | 74(1) |
| O(5) | 2945(3) | 2682(3) | 9281(3) | 102(1) |
| C(6) | 2127(4) | 453(4) | 6047(4) | 80(1) |
| O(6) | 1661(3) | 517(4) | 5283(3) | 110(1) |
| C(7) | 2105(3) | -790(4) | 7642(3) | 76(1) |
| O(7) | 1610(3) | -1500(3) | 7861(3) | 101(1) |
| C(8) | 3484(3) | 313(3) | 8591(4) | 74(1) |
| O(8) | 3866(3) | 279(3) | 9400(3) | 102(1) |
| C(9) | 3496(4) | 1589(5) | 6998(4) | 87(1) |
| O(9) | 3855(4) | 2372(4) | 6822(3) | 125(2) |
| C(10) | 4015(3) | -498(4) | 6645(4) | 88(2) |
| C(11) | 3796(3) | -1383(4) | 5979(4) | 80(1) |
| O(10) | 4630(3) | -1972(3) | 5646(3) | 106(1) |
| C(12) | 2920(5) | -1796(5) | 5598(5) | 92(2) |
| C(13) | 3199(6) | -2694(5) | 5017(5) | 108(2) |
| C(14) | 4224(6) | -2771(5) | 5074(5) | 111(2) |
| N(1) | 5023(8) | -187(14) | 6561(12) | 93(4) |
| C(15) | 5596(9) | 665(16) | 7044(15) | 115(5) |
| C(16) | 6677(8) | 401(11) | 7014(14) | 95(4) |
| C(17) | 7220(10) | 1037(13) | 7481(11) | 257(7) |
| N(1A) | 5041(11) | -611(12) | 6991(14) | 75(3) |
| C(15A) | 5636(10) | 108(13) | 7633(16) | 86(5) |
| C(16A) | 6784(19) | -80(20) | 7730(30) | 160(11) |
| C(17A) | 7220(10) | 1037(13) | 7481(11) | 257(7) |

**Table 3. Bond lengths [Å] and angles [º]**

| | | | |
|---|---|---|---|
| Mn(1)-C(1) | 1.798(5) | C(16)-H(16B) | 0.9700 |
| Mn(1)-C(5) | 1.840(5) | C(17)-H(17A) | 0.9600 |
| Mn(1)-C(4) | 1.842(5) | C(17)-H(17B) | 0.9600 |
| Mn(1)-C(2) | 1.843(6) | C(17)-H(17C) | 0.9600 |
| Mn(1)-C(3) | 1.852(6) | N(1A)-C(15A) | 1.453(19) |
| Mn(1)-Mn(2) | 2.9190(9) | N(1A)-H(1A) | 0.8600 |
| Mn(2)-C(8) | 1.828(5) | C(15A)-C(16A) | 1.49(3) |
| Mn(2)-C(7) | 1.828(6) | C(15A)-H(15C) | 0.9700 |
| Mn(2)-C(9) | 1.834(6) | C(15A)-H(15D) | 0.9700 |
| Mn(2)-C(6) | 1.845(5) | C(16A)-C(17A) | 1.58(3) |
| Mn(2)-C(10) | 1.994(5) | C(16A)-H(16C) | 0.9700 |
| C(1)-O(1) | 1.144(6) | C(16A)-H(16D) | 0.9700 |
| C(2)-O(2) | 1.142(6) | C(17A)-H(17D) | 0.9600 |
| C(3)-O(3) | 1.133(7) | C(17A)-H(17E) | 0.9600 |
| C(4)-O(4) | 1.133(5) | C(17A)-H(17F) | 0.9600 |
| C(5)-O(5) | 1.134(5) | | |
| C(6)-O(6) | 1.141(6) | C(1)-Mn(1)-C(5) | 93.6(2) |
| C(7)-O(7) | 1.150(6) | C(1)-Mn(1)-C(4) | 93.3(2) |
| C(8)-O(8) | 1.139(5) | C(5)-Mn(1)-C(4) | 90.5(2) |
| C(9)-O(9) | 1.137(6) | C(1)-Mn(1)-C(2) | 94.8(2) |
| C(10)-N(1) | 1.351(12) | C(5)-Mn(1)-C(2) | 90.2(2) |
| C(10)-N(1A) | 1.387(15) | C(4)-Mn(1)-C(2) | 171.9(2) |
| C(10)-C(11) | 1.454(6) | C(1)-Mn(1)-C(3) | 96.8(3) |
| C(11)-C(12) | 1.329(7) | C(5)-Mn(1)-C(3) | 169.6(2) |
| C(11)-O(10) | 1.376(6) | C(4)-Mn(1)-C(3) | 89.0(2) |
| O(10)-C(14) | 1.369(7) | C(2)-Mn(1)-C(3) | 88.9(3) |
| C(12)-C(13) | 1.424(8) | C(1)-Mn(1)-Mn(2) | 177.45(17) |
| C(12)-H(12) | 0.74(4) | C(5)-Mn(1)-Mn(2) | 84.13(13) |
| C(13)-C(14) | 1.312(9) | C(4)-Mn(1)-Mn(2) | 85.58(14) |
| C(13)-H(13) | 0.97(7) | C(2)-Mn(1)-Mn(2) | 86.44(17) |
| C(14)-H(14) | 0.93(7) | C(3)-Mn(1)-Mn(2) | 85.45(17) |
| N(1)-C(15) | 1.460(16) | C(8)-Mn(2)-C(7) | 89.2(2) |
| N(1)-H(1) | 0.8600 | C(8)-Mn(2)-C(9) | 91.1(2) |
| C(15)-C(16) | 1.420(16) | C(7)-Mn(2)-C(9) | 172.2(2) |
| C(15)-H(15A) | 0.9700 | C(8)-Mn(2)-C(6) | 173.3(2) |
| C(15)-H(15B) | 0.9700 | C(7)-Mn(2)-C(6) | 89.7(2) |
| C(16)-C(17) | 1.230(17) | C(9)-Mn(2)-C(6) | 89.2(2) |
| C(16)-H(16A) | 0.9700 | C(8)-Mn(2)-C(10) | 92.8(2) |

| | | | |
|---|---|---|---|
| C(7)-Mn(2)-C(10) | 92.7(2) | C(16)-C(15)-N(1) | 106.9(11) |
| C(9)-Mn(2)-C(10) | 95.0(2) | C(16)-C(15)-H(15A) | 110.3 |
| C(6)-Mn(2)-C(10) | 93.9(2) | N(1)-C(15)-H(15A) | 110.3 |
| C(8)-Mn(2)-Mn(1) | 85.83(14) | C(16)-C(15)-H(15B) | 110.3 |
| C(7)-Mn(2)-Mn(1) | 85.30(14) | N(1)-C(15)-H(15B) | 110.3 |
| C(9)-Mn(2)-Mn(1) | 86.97(16) | H(15A)-C(15)-H(15B) | 108.6 |
| C(6)-Mn(2)-Mn(1) | 87.47(15) | C(17)-C(16)-C(15) | 111.8(12) |
| C(10)-Mn(2)-Mn(1) | 177.59(18) | C(17)-C(16)-H(16A) | 109.3 |
| O(1)-C(1)-Mn(1) | 178.4(5) | C(15)-C(16)-H(16A) | 109.3 |
| O(2)-C(2)-Mn(1) | 177.8(5) | C(17)-C(16)-H(16B) | 109.3 |
| O(3)-C(3)-Mn(1) | 178.8(5) | C(15)-C(16)-H(16B) | 109.3 |
| O(4)-C(4)-Mn(1) | 177.8(4) | H(16A)-C(16)-H(16B) | 107.9 |
| O(5)-C(5)-Mn(1) | 179.8(4) | C(16)-C(17)-H(17A) | 109.5 |
| O(6)-C(6)-Mn(2) | 179.7(5) | C(16)-C(17)-H(17B) | 109.5 |
| O(7)-C(7)-Mn(2) | 179.2(5) | H(17A)-C(17)-H(17B) | 109.5 |
| O(8)-C(8)-Mn(2) | 179.1(4) | C(16)-C(17)-H(17C) | 109.5 |
| O(9)-C(9)-Mn(2) | 178.1(5) | H(17A)-C(17)-H(17C) | 109.5 |
| N(1)-C(10)-N(1A) | 32.9(5) | H(17B)-C(17)-H(17C) | 109.5 |
| N(1)-C(10)-C(11) | 111.9(6) | C(10)-N(1A)-C(15A) | 127.0(12) |
| N(1A)-C(10)-C(11) | 106.3(7) | C(10)-N(1A)-H(1A) | 116.5 |
| N(1)-C(10)-Mn(2) | 124.1(7) | C(15A)-N(1A)-H(1A) | 116.5 |
| N(1A)-C(10)-Mn(2) | 128.0(7) | N(1A)-C(15A)-C(16A) | 117.1(13) |
| C(11)-C(10)-Mn(2) | 122.2(3) | N(1A)-C(15A)-H(15C) | 108.0 |
| C(12)-C(11)-O(10) | 108.2(4) | C(16A)-C(15A)-H(15C) | 108.0 |
| C(12)-C(11)-C(10) | 133.8(5) | N(1A)-C(15A)-H(15D) | 108.0 |
| O(10)-C(11)-C(10) | 118.0(4) | C(16A)-C(15A)-H(15D) | 108.0 |
| C(14)-O(10)-C(11) | 107.0(5) | H(15C)-C(15A)-H(15D) | 107.3 |
| C(11)-C(12)-C(13) | 108.0(5) | C(15A)-C(16A)-C(17A) | 100(2) |
| C(11)-C(12)-H(12) | 127(3) | C(15A)-C(16A)-H(16C) | 111.7 |
| C(13)-C(12)-H(12) | 125(3) | C(17A)-C(16A)-H(16C) | 111.7 |
| C(14)-C(13)-C(12) | 106.4(6) | C(15A)-C(16A)-H(16D) | 111.7 |
| C(14)-C(13)-H(13) | 127(4) | C(17A)-C(16A)-H(16D) | 111.7 |
| C(12)-C(13)-H(13) | 125(4) | H(16C)-C(16A)-H(16D) | 109.5 |
| C(13)-C(14)-O(10) | 110.3(6) | C(16A)-C(17A)-H(17D) | 109.5 |
| C(13)-C(14)-H(14) | 132(4) | C(16A)-C(17A)-H(17E) | 109.5 |
| O(10)-C(14)-H(14) | 117(4) | H(17D)-C(17A)-H(17E) | 109.5 |
| C(10)-N(1)-C(15) | 131.9(10) | C(16A)-C(17A)-H(17F) | 109.5 |
| C(10)-N(1)-H(1) | 114.0 | H(17D)-C(17A)-H(17F) | 109.5 |
| C(15)-N(1)-H(1) | 114.0 | H(17E)-C(17A)-H(17F) | 109.5 |

**Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)**

The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Mn(1) | 56(1) | 93(1) | 56(1) | 3(1) | 6(1) | 7(1) |
| Mn(2) | 54(1) | 83(1) | 64(1) | -12(1) | 6(1) | -4(1) |
| C(1) | 66(3) | 136(5) | 80(3) | 6(3) | 5(2) | 24(3) |
| O(1) | 88(3) | 181(4) | 124(3) | -10(3) | 18(2) | 58(3) |
| C(2) | 91(3) | 116(4) | 68(3) | 4(3) | 0(2) | 14(3) |
| O(2) | 165(4) | 147(4) | 83(2) | 39(3) | 5(3) | 20(3) |
| C(3) | 62(3) | 136(5) | 85(3) | 1(3) | -1(2) | 1(3) |
| O(3) | 85(3) | 197(5) | 134(4) | -32(3) | -18(3) | -23(3) |
| C(4) | 64(3) | 98(3) | 65(2) | -1(2) | 9(2) | 0(2) |
| O(4) | 112(3) | 120(3) | 80(2) | 28(2) | 12(2) | 3(2) |
| C(5) | 66(3) | 86(3) | 70(2) | -3(2) | 13(2) | 8(2) |
| O(5) | 81(2) | 117(3) | 107(3) | -29(2) | 2(2) | -9(2) |
| C(6) | 75(3) | 94(3) | 70(3) | -10(2) | 10(2) | -6(2) |
| O(6) | 120(3) | 140(4) | 70(2) | -1(2) | -13(2) | -1(3) |
| C(7) | 68(3) | 95(3) | 66(2) | -13(2) | 0(2) | 0(3) |
| O(7) | 104(3) | 101(3) | 98(3) | 0(2) | 10(2) | -24(2) |
| C(8) | 65(2) | 74(3) | 83(3) | -13(2) | -6(2) | 0(2) |
| O(8) | 100(3) | 111(3) | 94(2) | -1(2) | -30(2) | 1(2) |
| C(9) | 73(3) | 111(4) | 78(3) | -15(3) | 22(2) | -18(3) |
| O(9) | 131(4) | 126(3) | 116(3) | -2(3) | 39(3) | -47(3) |
| C(10) | 57(2) | 110(4) | 98(3) | -37(3) | 4(2) | -7(2) |
| C(11) | 63(3) | 95(3) | 82(3) | -21(2) | 7(2) | -1(2) |
| O(10) | 79(2) | 118(3) | 120(3) | -32(2) | 9(2) | 16(2) |
| C(12) | 67(3) | 112(4) | 98(4) | -31(3) | 5(3) | -6(3) |
| C(13) | 107(5) | 115(5) | 101(4) | -36(4) | 3(3) | -18(4) |
| C(14) | 121(5) | 98(4) | 113(4) | -33(4) | 22(4) | 2(4) |
| N(1) | 56(4) | 118(11) | 104(8) | -35(7) | 1(5) | -2(6) |
| C(15) | 72(6) | 148(13) | 127(11) | -32(10) | -7(6) | -26(7) |
| C(16) | 60(5) | 99(8) | 125(9) | -23(7) | 3(5) | -31(5) |
| C(17) | 207(13) | 258(17) | 307(19) | -22(15) | 91(13) | 36(12) |
| N(1A) | 54(5) | 68(7) | 102(10) | -3(6) | -5(6) | 1(5) |
| C(15A) | 63(7) | 82(9) | 113(11) | -9(8) | -6(7) | -12(6) |
| C(16A) | 170(20) | 150(20) | 170(20) | -65(18) | -4(16) | -71(16) |
| C(17A) | 207(13) | 258(17) | 307(19) | -22(15) | 91(13) | 36(12) |

**Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$x $10^3$)**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(12) | 2380(30) | -1610(30) | 5680(30) | 57(13) |
| H(13) | 2730(60) | -3070(50) | 4550(50) | 140(20) |
| H(14) | 4700(50) | -3260(50) | 4820(50) | 130(20) |
| H(1) | 5397 | -560 | 6145 | 111 |
| H(15A) | 5473 | 1297 | 6656 | 139 |
| H(15B) | 5368 | 764 | 7765 | 139 |
| H(16A) | 6774 | -271 | 7333 | 114 |
| H(16B) | 6905 | 358 | 6286 | 114 |
| H(17A) | 7945 | 841 | 7434 | 386 |
| H(17B) | 7013 | 1063 | 8208 | 386 |
| H(17C) | 7125 | 1703 | 7167 | 386 |
| H(1A) | 5360 | -1166 | 6804 | 90 |
| H(15C) | 5336 | 106 | 8336 | 103 |
| H(15D) | 5537 | 793 | 7346 | 103 |
| H(16C) | 7029 | -583 | 7224 | 192 |
| H(16D) | 6973 | -302 | 8437 | 192 |
| H(17D) | 7973 | 1019 | 7461 | 386 |
| H(17E) | 6995 | 1507 | 8020 | 386 |
| H(17F) | 6956 | 1262 | 6812 | 386 |

**Table 6. Torsion angles [º]**

| | | | |
|---|---|---|---|
| C(5)-Mn(1)-Mn(2)-C(8) | 45.6(2) | C(2)-Mn(1)-Mn(2)-C(6) | -44.5(2) |
| C(4)-Mn(1)-Mn(2)-C(8) | -45.4(2) | C(3)-Mn(1)-Mn(2)-C(6) | 44.6(2) |
| C(2)-Mn(1)-Mn(2)-C(8) | 136.1(2) | C(8)-Mn(2)-C(10)-N(1) | -64.8(11) |
| C(3)-Mn(1)-Mn(2)-C(8) | -134.7(2) | C(7)-Mn(2)-C(10)-N(1) | -154.2(11) |
| C(5)-Mn(1)-Mn(2)-C(7) | 135.1(2) | C(9)-Mn(2)-C(10)-N(1) | 26.5(11) |
| C(4)-Mn(1)-Mn(2)-C(7) | 44.1(2) | C(6)-Mn(2)-C(10)-N(1) | 116.0(11) |
| C(2)-Mn(1)-Mn(2)-C(7) | -134.3(2) | C(8)-Mn(2)-C(10)-N(1A) | -24.1(11) |
| C(3)-Mn(1)-Mn(2)-C(7) | -45.2(2) | C(7)-Mn(2)-C(10)-N(1A) | -113.5(10) |
| C(5)-Mn(1)-Mn(2)-C(9) | -45.8(2) | C(9)-Mn(2)-C(10)-N(1A) | 67.2(11) |
| C(4)-Mn(1)-Mn(2)-C(9) | -136.7(2) | C(6)-Mn(2)-C(10)-N(1A) | 156.7(10) |
| C(2)-Mn(1)-Mn(2)-C(9) | 44.8(2) | C(8)-Mn(2)-C(10)-C(11) | 131.8(5) |
| C(3)-Mn(1)-Mn(2)-C(9) | 133.9(3) | C(7)-Mn(2)-C(10)-C(11) | 42.5(5) |
| C(5)-Mn(1)-Mn(2)-C(6) | -135.1(2) | C(9)-Mn(2)-C(10)-C(11) | -136.8(5) |
| C(4)-Mn(1)-Mn(2)-C(6) | 134.0(2) | C(6)-Mn(2)-C(10)-C(11) | -47.3(5) |

| | | | |
|---|---|---|---|
| N(1)-C(10)-C(11)-C(12) | -160.6(11) | C(12)-C(13)-C(14)-O(10) | -0.7(8) |
| N(1A)-C(10)-C(11)-C(12) | 165.0(10) | C(11)-O(10)-C(14)-C(13) | 1.4(8) |
| Mn(2)-C(10)-C(11)-C(12) | 4.5(10) | C(11)-C(10)-N(1)-C(15) | 178.3(13) |
| N(1)-C(10)-C(11)-O(10) | 20.4(12) | Mn(2)-C(10)-N(1)-C(15) | 13(2) |
| N(1A)-C(10)-C(11)-O(10) | -14.0(10) | C(10)-N(1)-C(15)-C(16) | 157.6(17) |
| Mn(2)-C(10)-C(11)-O(10) | -174.4(4) | N(1)-C(15)-C(16)-C(17) | -174.5(16) |
| C(12)-C(11)-O(10)-C(14) | -1.6(7) | N(1)-C(10)-N(1A)-C(15A) | 71.4(17) |
| C(10)-C(11)-O(10)-C(14) | 177.6(5) | C(11)-C(10)-N(1A)-C(15A) | 176.6(12) |
| O(10)-C(11)-C(12)-C(13) | 1.2(7) | Mn(2)-C(10)-N(1A)-C(15A) | -24.5(18) |
| C(10)-C(11)-C(12)-C(13) | -177.9(6) | C(10)-N(1A)-C(15A)-C(16A) | -168.4(15) |
| C(11)-C(12)-C(13)-C(14) | -0.3(8) | N(1A)-C(15A)-C(16A)-C(17A) | 131.1(15) |