**Table S1.** Crystal data and structure refinement for Complex **10** mo_IALVB88_0m_aa.

| | | |
|---|---|---|
| Identification code | mo_IALVB88_0m_aa | |
| Empirical formula | C45 H30 Eu F12 N O8 | |
| Formula weight | 1092.66 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/n | |
| Unit cell dimensions | a = 11.1009(6) Å | α= 90°. |
| | b = 21.8025(12) Å | β= 106.930(3)°. |
| | c = 18.7796(11) Å | γ = 90°. |
| Volume | 4348.2(4) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.669 $Mg/m^3$ | |
| Absorption coefficient | 1.549 $mm^{-1}$ | |
| F(000) | 2168 | |
| Crystal size | 0.295 x 0.079 x 0.038 $mm^3$ | |
| Theta range for data collection | 2.267 to 24.999°. | |
| Index ranges | -12<=h<=12, 0<=k<=25, 0<=l<=22 | |
| Reflections collected | 6112 | |
| Independent reflections | 6112 [R(int) = 0.1366] | |
| Completeness to theta = 24.999° | 80.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7461 and 0.4731 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 6112 / 1 / 568 | |
| Goodness-of-fit on $F^2$ | 0.832 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0324, wR2 = 0.0438 | |
| R indices (all data) | R1 = 0.0824, wR2 = 0.0505 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 1.069 and -0.807 $e.Å^{-3}$ | |

**Table S2**. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for mo_IALVB88_0m_aa. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Eu(1) | 7927(1) | 6864(1) | 3143(1) | 15(1) |
| F(1) | 5397(3) | 5274(1) | 3769(2) | 36(1) |
| F(2) | 5141(3) | 5903(1) | 4591(2) | 36(1) |
| F(3) | 6334(3) | 5112(1) | 4927(2) | 41(1) |
| F(4) | 5092(4) | 5957(2) | 894(2) | 67(2) |
| F(5) | 4784(5) | 5253(2) | 1601(2) | 86(2) |
| F(6) | 5860(3) | 5072(1) | 853(2) | 41(1) |
| F(7) | 7402(4) | 7339(1) | 63(2) | 45(1) |
| F(8) | 9215(4) | 7358(2) | 859(2) | 56(1) |
| F(9) | 8212(4) | 6511(2) | 602(2) | 58(2) |
| F(10) | 10542(4) | 8741(2) | 2832(2) | 69(2) |
| F(11) | 11804(3) | 8150(1) | 3582(1) | 34(1) |
| F(12) | 11228(4) | 8949(2) | 4003(2) | 69(2) |
| O(1) | 6729(3) | 6359(1) | 3835(2) | 19(1) |
| O(2) | 9342(3) | 6586(1) | 4335(2) | 16(1) |
| O(3) | 6536(3) | 6113(1) | 2328(2) | 19(1) |
| O(4) | 9134(3) | 6022(1) | 2977(2) | 19(1) |
| O(5) | 8252(3) | 7042(1) | 1971(2) | 20(1) |
| O(6) | 6124(3) | 7385(1) | 2407(2) | 18(1) |
| O(7) | 9556(3) | 7613(1) | 3347(2) | 18(1) |
| O(8) | 7423(3) | 7666(1) | 3851(2) | 17(1) |
| C(1) | 6020(7) | 5550(3) | 4408(3) | 28(2) |
| C(2) | 7082(6) | 5940(2) | 4327(3) | 17(2) |
| C(3) | 8266(5) | 5813(2) | 4783(3) | 20(2) |
| C(4) | 9342(5) | 6176(2) | 4799(3) | 18(2) |
| C(5) | 10563(6) | 6063(2) | 5393(3) | 22(2) |
| C(6) | 10533(6) | 5867(2) | 6109(3) | 36(2) |
| C(7) | 11679(7) | 5794(3) | 6657(3) | 47(3) |
| C(8) | 12780(7) | 5908(3) | 6491(4) | 46(3) |
| C(9) | 12817(7) | 6114(2) | 5797(3) | 44(3) |
| C(10) | 11668(6) | 6193(2) | 5248(3) | 29(2) |
| C(11) | 5624(7) | 5488(3) | 1323(3) | 35(2) |

| | | | | |
|---|---|---|---|---|
| C(12) | 6796(5) | 5708(2) | 1912(3) | 16(2) |
| C(13) | 7923(5) | 5455(2) | 1945(3) | 15(2) |
| C(14) | 9105(5) | 5621(2) | 2491(2) | 12(2) |
| C(15) | 10287(5) | 5301(2) | 2516(3) | 12(2) |
| C(16) | 10495(6) | 4982(2) | 1914(3) | 21(2) |
| C(17) | 11635(6) | 4748(2) | 1972(3) | 28(2) |
| C(18) | 12666(6) | 4813(2) | 2616(3) | 23(2) |
| C(19) | 12434(6) | 5114(2) | 3220(3) | 23(2) |
| C(20) | 11278(5) | 5356(2) | 3173(3) | 20(2) |
| C(21) | 8080(7) | 7116(3) | 715(3) | 29(2) |
| C(22) | 7503(6) | 7202(2) | 1346(3) | 19(1) |
| C(23) | 6278(6) | 7402(2) | 1182(3) | 19(1) |
| C(24) | 5655(5) | 7491(2) | 1718(3) | 12(2) |
| C(25) | 4312(5) | 7729(2) | 1488(3) | 16(2) |
| C(26) | 3513(6) | 7645(2) | 758(3) | 21(2) |
| C(27) | 2291(6) | 7855(2) | 583(3) | 25(2) |
| C(28) | 1856(6) | 8155(2) | 1103(3) | 32(2) |
| C(29) | 2658(5) | 8251(2) | 1816(3) | 30(2) |
| C(30) | 3862(6) | 8025(2) | 2008(3) | 21(2) |
| C(31) | 10797(7) | 8492(3) | 3503(4) | 35(2) |
| C(32) | 9674(6) | 8147(3) | 3601(2) | 23(2) |
| C(33) | 8904(6) | 8458(2) | 3927(3) | 26(2) |
| C(34) | 7774(5) | 8212(2) | 4028(2) | 16(2) |
| C(35) | 6945(6) | 8579(2) | 4357(2) | 19(2) |
| C(36) | 7376(6) | 9109(2) | 4789(2) | 17(2) |
| C(37) | 6562(6) | 9404(2) | 5109(3) | 24(2) |
| C(38) | 5348(6) | 9192(2) | 5010(3) | 27(2) |
| C(39) | 4922(6) | 8685(2) | 4557(2) | 23(2) |
| C(40) | 5720(6) | 8387(2) | 4245(3) | 16(2) |
| N(1) | 3954(6) | 6660(2) | 3143(3) | 50(1) |
| C(41) | 3967(7) | 6446(2) | 2471(3) | 50(1) |
| C(42) | 2958(7) | 6431(2) | 1921(4) | 50(1) |
| C(43) | 1909(8) | 6613(2) | 1983(4) | 50(1) |
| C(44) | 1791(7) | 6833(3) | 2569(3) | 50(1) |
| C(45) | 2701(6) | 6882(3) | 3240(3) | 50(1) |

**Table S3.** Bond lengths [Å] and angles [°] for mo_IALVB88_0m_aa.

| | |
|---|---|
| Eu(1)-O(4) | 2.347(3) |
| Eu(1)-O(8) | 2.360(3) |
| Eu(1)-O(5) | 2.364(4) |
| Eu(1)-O(6) | 2.366(3) |
| Eu(1)-O(1) | 2.381(4) |
| Eu(1)-O(7) | 2.384(3) |
| Eu(1)-O(2) | 2.408(3) |
| Eu(1)-O(3) | 2.455(3) |
| F(1)-C(1) | 1.341(5) |
| F(2)-C(1) | 1.363(8) |
| F(3)-C(1) | 1.337(5) |
| F(4)-C(11) | 1.329(6) |
| F(5)-C(11) | 1.299(9) |
| F(6)-C(11) | 1.344(7) |
| F(7)-C(21) | 1.329(6) |
| F(8)-C(21) | 1.318(8) |
| F(9)-C(21) | 1.353(6) |
| F(10)-C(31) | 1.324(7) |
| F(11)-C(31) | 1.315(7) |
| F(12)-C(31) | 1.359(6) |
| O(1)-C(2) | 1.278(5) |
| O(2)-C(4) | 1.248(5) |
| O(3)-C(12) | 1.268(6) |
| O(4)-C(14) | 1.258(5) |
| O(5)-C(22) | 1.275(5) |
| O(6)-C(24) | 1.267(5) |
| O(7)-C(32) | 1.249(6) |
| O(8)-C(34) | 1.267(5) |
| C(1)-C(2) | 1.496(9) |
| C(2)-C(3) | 1.371(6) |
| C(3)-C(4) | 1.426(8) |
| C(3)-H(3) | 0.9500 |
| C(4)-C(5) | 1.504(6) |
| C(5)-C(10) | 1.361(9) |

| | |
|---|---|
| C(5)-C(6) | 1.420(8) |
| C(6)-C(7) | 1.393(7) |
| C(6)-H(6) | 0.9500 |
| C(7)-C(8) | 1.368(11) |
| C(7)-H(7) | 0.9500 |
| C(8)-C(9) | 1.392(9) |
| C(8)-H(8) | 0.9500 |
| C(9)-C(10) | 1.398(7) |
| C(9)-H(9) | 0.9500 |
| C(10)-H(10) | 0.9500 |
| C(11)-C(12) | 1.519(7) |
| C(12)-C(13) | 1.353(8) |
| C(13)-C(14) | 1.456(6) |
| C(13)-H(13) | 0.9500 |
| C(14)-C(15) | 1.475(8) |
| C(15)-C(20) | 1.399(6) |
| C(15)-C(16) | 1.401(7) |
| C(16)-C(17) | 1.339(8) |
| C(16)-H(16) | 0.9500 |
| C(17)-C(18) | 1.409(6) |
| C(17)-H(17) | 0.9500 |
| C(18)-C(19) | 1.398(7) |
| C(18)-H(18) | 0.9500 |
| C(19)-C(20) | 1.367(8) |
| C(19)-H(19) | 0.9500 |
| C(20)-H(20) | 0.9500 |
| C(21)-C(22) | 1.513(10) |
| C(22)-C(23) | 1.375(9) |
| C(23)-C(24) | 1.392(8) |
| C(23)-H(23) | 0.9500 |
| C(24)-C(25) | 1.517(6) |
| C(25)-C(30) | 1.380(8) |
| C(25)-C(26) | 1.410(5) |
| C(26)-C(27) | 1.378(9) |
| C(26)-H(26) | 0.9500 |
| C(27)-C(28) | 1.374(8) |

| | |
|---|---|
| C(27)-H(27) | 0.9500 |
| C(28)-C(29) | 1.392(5) |
| C(28)-H(28) | 0.9500 |
| C(29)-C(30) | 1.370(8) |
| C(29)-H(29) | 0.9500 |
| C(30)-H(30) | 0.9500 |
| C(31)-C(32) | 1.512(10) |
| C(32)-C(33) | 1.368(9) |
| C(33)-C(34) | 1.426(9) |
| C(33)-H(33) | 0.9500 |
| C(34)-C(35) | 1.483(8) |
| C(35)-C(40) | 1.379(8) |
| C(35)-C(36) | 1.413(6) |
| C(36)-C(37) | 1.381(8) |
| C(36)-H(36) | 0.9500 |
| C(37)-C(38) | 1.386(9) |
| C(37)-H(37) | 0.9500 |
| C(38)-C(39) | 1.389(6) |
| C(38)-H(38) | 0.9500 |
| C(39)-C(40) | 1.362(8) |
| C(39)-H(39) | 0.9500 |
| C(40)-H(40) | 0.9500 |
| N(1)-C(41) | 1.350(8) |
| N(1)-C(45) | 1.533(9) |
| N(1)-H(1A) | 0.8800 |
| C(41)-C(42) | 1.284(7) |
| C(41)-H(41) | 0.9500 |
| C(42)-C(43) | 1.267(11) |
| C(42)-H(42) | 0.9500 |
| C(43)-C(44) | 1.242(9) |
| C(43)-H(43) | 0.9500 |
| C(44)-C(45) | 1.371(6) |
| C(44)-H(44) | 0.9500 |
| C(45)-H(45) | 0.9500 |

| | |
|---|---|
| O(4)-Eu(1)-O(8) | 153.22(9) |

| | |
|---|---|
| O(4)-Eu(1)-O(5) | 75.95(11) |
| O(8)-Eu(1)-O(5) | 121.84(10) |
| O(4)-Eu(1)-O(6) | 135.81(10) |
| O(8)-Eu(1)-O(6) | 70.97(10) |
| O(5)-Eu(1)-O(6) | 73.12(12) |
| O(4)-Eu(1)-O(1) | 98.17(13) |
| O(8)-Eu(1)-O(1) | 76.94(12) |
| O(5)-Eu(1)-O(1) | 147.63(10) |
| O(6)-Eu(1)-O(1) | 91.65(12) |
| O(4)-Eu(1)-O(7) | 96.98(13) |
| O(8)-Eu(1)-O(7) | 72.23(13) |
| O(5)-Eu(1)-O(7) | 73.89(11) |
| O(6)-Eu(1)-O(7) | 103.76(11) |
| O(1)-Eu(1)-O(7) | 138.33(10) |
| O(4)-Eu(1)-O(2) | 71.53(11) |
| O(8)-Eu(1)-O(2) | 82.00(10) |
| O(5)-Eu(1)-O(2) | 132.21(13) |
| O(6)-Eu(1)-O(2) | 151.16(12) |
| O(1)-Eu(1)-O(2) | 72.14(12) |
| O(7)-Eu(1)-O(2) | 76.36(10) |
| O(4)-Eu(1)-O(3) | 71.06(11) |
| O(8)-Eu(1)-O(3) | 129.49(13) |
| O(5)-Eu(1)-O(3) | 76.58(12) |
| O(6)-Eu(1)-O(3) | 71.62(10) |
| O(1)-Eu(1)-O(3) | 71.49(11) |
| O(7)-Eu(1)-O(3) | 150.09(12) |
| O(2)-Eu(1)-O(3) | 122.22(10) |
| C(2)-O(1)-Eu(1) | 128.5(4) |
| C(4)-O(2)-Eu(1) | 134.2(3) |
| C(12)-O(3)-Eu(1) | 129.4(4) |
| C(14)-O(4)-Eu(1) | 138.2(3) |
| C(22)-O(5)-Eu(1) | 131.9(4) |
| C(24)-O(6)-Eu(1) | 135.2(3) |
| C(32)-O(7)-Eu(1) | 133.6(4) |
| C(34)-O(8)-Eu(1) | 137.7(4) |
| F(3)-C(1)-F(1) | 106.8(4) |

| | |
|---|---|
| F(3)-C(1)-F(2) | 105.9(6) |
| F(1)-C(1)-F(2) | 105.0(5) |
| F(3)-C(1)-C(2) | 115.7(5) |
| F(1)-C(1)-C(2) | 112.3(5) |
| F(2)-C(1)-C(2) | 110.4(5) |
| O(1)-C(2)-C(3) | 129.2(5) |
| O(1)-C(2)-C(1) | 113.3(4) |
| C(3)-C(2)-C(1) | 117.5(5) |
| C(2)-C(3)-C(4) | 123.1(5) |
| C(2)-C(3)-H(3) | 118.5 |
| C(4)-C(3)-H(3) | 118.5 |
| O(2)-C(4)-C(3) | 123.6(4) |
| O(2)-C(4)-C(5) | 116.9(5) |
| C(3)-C(4)-C(5) | 119.5(5) |
| C(10)-C(5)-C(6) | 121.5(5) |
| C(10)-C(5)-C(4) | 119.2(5) |
| C(6)-C(5)-C(4) | 119.2(7) |
| C(7)-C(6)-C(5) | 117.7(7) |
| C(7)-C(6)-H(6) | 121.1 |
| C(5)-C(6)-H(6) | 121.1 |
| C(8)-C(7)-C(6) | 119.7(7) |
| C(8)-C(7)-H(7) | 120.1 |
| C(6)-C(7)-H(7) | 120.1 |
| C(7)-C(8)-C(9) | 122.9(6) |
| C(7)-C(8)-H(8) | 118.5 |
| C(9)-C(8)-H(8) | 118.5 |
| C(8)-C(9)-C(10) | 117.4(8) |
| C(8)-C(9)-H(9) | 121.3 |
| C(10)-C(9)-H(9) | 121.3 |
| C(5)-C(10)-C(9) | 120.6(6) |
| C(5)-C(10)-H(10) | 119.7 |
| C(9)-C(10)-H(10) | 119.7 |
| F(5)-C(11)-F(4) | 107.6(7) |
| F(5)-C(11)-F(6) | 107.3(5) |
| F(4)-C(11)-F(6) | 105.0(5) |
| F(5)-C(11)-C(12) | 113.2(6) |

| | |
|---|---|
| F(4)-C(11)-C(12) | 109.5(5) |
| F(6)-C(11)-C(12) | 113.7(6) |
| O(3)-C(12)-C(13) | 129.0(4) |
| O(3)-C(12)-C(11) | 111.7(5) |
| C(13)-C(12)-C(11) | 119.3(5) |
| C(12)-C(13)-C(14) | 124.3(5) |
| C(12)-C(13)-H(13) | 117.9 |
| C(14)-C(13)-H(13) | 117.9 |
| O(4)-C(14)-C(13) | 120.7(5) |
| O(4)-C(14)-C(15) | 118.1(4) |
| C(13)-C(14)-C(15) | 121.1(4) |
| C(20)-C(15)-C(16) | 118.9(5) |
| C(20)-C(15)-C(14) | 116.8(5) |
| C(16)-C(15)-C(14) | 124.2(4) |
| C(17)-C(16)-C(15) | 119.8(5) |
| C(17)-C(16)-H(16) | 120.1 |
| C(15)-C(16)-H(16) | 120.1 |
| C(16)-C(17)-C(18) | 122.9(6) |
| C(16)-C(17)-H(17) | 118.5 |
| C(18)-C(17)-H(17) | 118.5 |
| C(19)-C(18)-C(17) | 116.6(6) |
| C(19)-C(18)-H(18) | 121.7 |
| C(17)-C(18)-H(18) | 121.7 |
| C(20)-C(19)-C(18) | 121.3(5) |
| C(20)-C(19)-H(19) | 119.3 |
| C(18)-C(19)-H(19) | 119.3 |
| C(19)-C(20)-C(15) | 120.4(5) |
| C(19)-C(20)-H(20) | 119.8 |
| C(15)-C(20)-H(20) | 119.8 |
| F(8)-C(21)-F(7) | 107.1(6) |
| F(8)-C(21)-F(9) | 106.3(7) |
| F(7)-C(21)-F(9) | 105.6(5) |
| F(8)-C(21)-C(22) | 112.8(5) |
| F(7)-C(21)-C(22) | 114.9(6) |
| F(9)-C(21)-C(22) | 109.6(5) |
| O(5)-C(22)-C(23) | 129.1(6) |

| | |
|---|---|
| O(5)-C(22)-C(21) | 112.1(6) |
| C(23)-C(22)-C(21) | 118.7(5) |
| C(22)-C(23)-C(24) | 123.3(5) |
| C(22)-C(23)-H(23) | 118.3 |
| C(24)-C(23)-H(23) | 118.3 |
| O(6)-C(24)-C(23) | 124.8(5) |
| O(6)-C(24)-C(25) | 115.5(5) |
| C(23)-C(24)-C(25) | 119.7(4) |
| C(30)-C(25)-C(26) | 119.5(5) |
| C(30)-C(25)-C(24) | 119.1(4) |
| C(26)-C(25)-C(24) | 121.4(5) |
| C(27)-C(26)-C(25) | 119.1(6) |
| C(27)-C(26)-H(26) | 120.5 |
| C(25)-C(26)-H(26) | 120.5 |
| C(28)-C(27)-C(26) | 120.9(5) |
| C(28)-C(27)-H(27) | 119.5 |
| C(26)-C(27)-H(27) | 119.5 |
| C(27)-C(28)-C(29) | 119.8(6) |
| C(27)-C(28)-H(28) | 120.1 |
| C(29)-C(28)-H(28) | 120.1 |
| C(30)-C(29)-C(28) | 120.0(6) |
| C(30)-C(29)-H(29) | 120.0 |
| C(28)-C(29)-H(29) | 120.0 |
| C(29)-C(30)-C(25) | 120.6(5) |
| C(29)-C(30)-H(30) | 119.7 |
| C(25)-C(30)-H(30) | 119.7 |
| F(11)-C(31)-F(10) | 106.2(7) |
| F(11)-C(31)-F(12) | 102.7(5) |
| F(10)-C(31)-F(12) | 106.9(5) |
| F(11)-C(31)-C(32) | 114.1(5) |
| F(10)-C(31)-C(32) | 111.4(5) |
| F(12)-C(31)-C(32) | 114.7(6) |
| O(7)-C(32)-C(33) | 128.5(6) |
| O(7)-C(32)-C(31) | 114.6(6) |
| C(33)-C(32)-C(31) | 116.9(6) |
| C(32)-C(33)-C(34) | 124.2(6) |

| | |
|---|---|
| C(32)-C(33)-H(33) | 117.9 |
| C(34)-C(33)-H(33) | 117.9 |
| O(8)-C(34)-C(33) | 122.2(6) |
| O(8)-C(34)-C(35) | 115.8(6) |
| C(33)-C(34)-C(35) | 122.1(5) |
| C(40)-C(35)-C(36) | 119.4(6) |
| C(40)-C(35)-C(34) | 118.5(5) |
| C(36)-C(35)-C(34) | 122.2(6) |
| C(37)-C(36)-C(35) | 118.4(6) |
| C(37)-C(36)-H(36) | 120.8 |
| C(35)-C(36)-H(36) | 120.8 |
| C(36)-C(37)-C(38) | 121.3(5) |
| C(36)-C(37)-H(37) | 119.4 |
| C(38)-C(37)-H(37) | 119.4 |
| C(37)-C(38)-C(39) | 119.5(6) |
| C(37)-C(38)-H(38) | 120.3 |
| C(39)-C(38)-H(38) | 120.3 |
| C(40)-C(39)-C(38) | 119.7(6) |
| C(40)-C(39)-H(39) | 120.2 |
| C(38)-C(39)-H(39) | 120.2 |
| C(39)-C(40)-C(35) | 121.7(5) |
| C(39)-C(40)-H(40) | 119.2 |
| C(35)-C(40)-H(40) | 119.2 |
| C(41)-N(1)-C(45) | 118.5(6) |
| C(41)-N(1)-H(1A) | 120.7 |
| C(45)-N(1)-H(1A) | 120.7 |
| C(42)-C(41)-N(1) | 121.1(8) |
| C(42)-C(41)-H(41) | 119.5 |
| N(1)-C(41)-H(41) | 119.5 |
| C(43)-C(42)-C(41) | 121.9(8) |
| C(43)-C(42)-H(42) | 119.1 |
| C(41)-C(42)-H(42) | 119.1 |
| C(44)-C(43)-C(42) | 122.6(8) |
| C(44)-C(43)-H(43) | 118.7 |
| C(42)-C(43)-H(43) | 118.7 |
| C(43)-C(44)-C(45) | 127.2(8) |

| | |
|---|---|
| C(43)-C(44)-H(44) | 116.4 |
| C(45)-C(44)-H(44) | 116.4 |
| C(44)-C(45)-N(1) | 108.5(5) |
| C(44)-C(45)-H(45) | 125.7 |
| N(1)-C(45)-H(45) | 125.7 |

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Symmetry transformations used to generate equivalent atoms:

**Table S4.** Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_IALVB88_0m_aa. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Eu(1) | 11(1) | 16(1) | 18(1) | -1(1) | 7(1) | 0(1) |
| F(1) | 33(3) | 34(2) | 42(2) | -4(2) | 9(2) | -9(2) |
| F(2) | 33(3) | 40(2) | 39(2) | 4(2) | 15(2) | -3(2) |
| F(3) | 32(3) | 37(2) | 54(2) | 15(2) | 10(2) | -6(2) |
| F(4) | 52(4) | 57(3) | 71(3) | -10(2) | -17(3) | 9(2) |
| F(5) | 66(5) | 104(4) | 90(3) | -42(3) | 26(3) | -36(3) |
| F(6) | 24(3) | 49(2) | 48(2) | -20(2) | 4(2) | -1(2) |
| F(7) | 43(3) | 61(2) | 33(2) | 4(2) | 16(2) | 5(2) |
| F(8) | 43(4) | 82(3) | 50(2) | 0(2) | 23(2) | -7(2) |
| F(9) | 78(4) | 50(3) | 61(2) | -4(2) | 44(2) | 11(2) |
| F(10) | 29(4) | 104(3) | 81(3) | 51(2) | 25(3) | 1(2) |
| F(11) | 19(2) | 44(2) | 40(2) | 4(2) | 12(2) | -4(2) |
| F(12) | 56(4) | 62(3) | 104(3) | -25(2) | 45(3) | -15(2) |
| O(1) | 15(3) | 17(2) | 25(2) | 2(2) | 7(2) | 2(2) |
| O(2) | 13(3) | 21(2) | 16(2) | 1(2) | 9(2) | -5(2) |
| O(3) | 14(3) | 17(2) | 24(2) | -6(2) | 4(2) | 1(2) |
| O(4) | 11(3) | 25(2) | 20(2) | -3(2) | 5(2) | 5(2) |
| O(5) | 13(3) | 26(2) | 26(2) | 3(2) | 12(2) | 2(2) |
| O(6) | 17(3) | 23(2) | 17(2) | 2(2) | 9(2) | 2(2) |
| O(7) | 16(3) | 20(2) | 23(2) | -2(2) | 12(2) | -4(2) |
| O(8) | 18(3) | 18(2) | 16(2) | -3(2) | 6(2) | 0(2) |
| C(1) | 27(5) | 19(3) | 39(4) | 3(3) | 10(4) | 2(3) |
| C(2) | 16(4) | 14(3) | 22(3) | -3(2) | 7(3) | -1(3) |
| C(3) | 18(4) | 16(3) | 29(3) | -1(2) | 10(3) | -5(3) |
| C(4) | 12(4) | 25(3) | 18(3) | -10(2) | 3(3) | 0(3) |
| C(5) | 21(5) | 19(3) | 24(3) | -3(2) | 4(3) | -1(3) |
| C(6) | 35(6) | 33(4) | 39(3) | 9(3) | 9(4) | 0(3) |
| C(7) | 44(6) | 43(4) | 42(4) | 10(3) | -3(5) | 3(4) |
| C(8) | 21(6) | 51(5) | 58(5) | 3(4) | 0(5) | 10(4) |
| C(9) | 31(6) | 39(4) | 58(4) | -10(3) | 5(4) | 4(3) |
| C(10) | 20(5) | 29(3) | 35(3) | -1(3) | 3(4) | -2(3) |
| C(11) | 36(6) | 27(4) | 37(4) | -16(3) | 4(4) | -3(4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(12) | 9(5) | 16(3) | 22(3) | 0(2) | 2(3) | -3(3) |
| C(13) | 13(4) | 11(3) | 18(3) | -4(2) | 2(3) | 4(2) |
| C(14) | 15(4) | 13(3) | 12(3) | 2(2) | 7(3) | 2(3) |
| C(15) | 11(4) | 14(3) | 14(3) | 1(2) | 8(3) | 6(3) |
| C(16) | 18(5) | 25(3) | 17(3) | 3(2) | 2(3) | 3(3) |
| C(17) | 36(6) | 21(3) | 28(3) | 3(3) | 12(4) | 0(3) |
| C(18) | 20(5) | 23(3) | 28(3) | 1(3) | 12(3) | 6(3) |
| C(19) | 16(5) | 23(3) | 28(3) | 0(3) | 4(3) | 1(3) |
| C(20) | 22(5) | 19(3) | 20(3) | -5(2) | 9(3) | 3(3) |
| C(21) | 27(6) | 38(4) | 31(4) | 3(3) | 22(4) | -2(3) |
| C(22) | 20(3) | 20(2) | 22(2) | 0(2) | 15(2) | -1(2) |
| C(23) | 20(3) | 20(2) | 22(2) | 0(2) | 15(2) | -1(2) |
| C(24) | 11(4) | 10(3) | 19(3) | -1(2) | 11(3) | -2(2) |
| C(25) | 17(4) | 14(3) | 19(3) | 2(2) | 9(3) | 2(3) |
| C(26) | 26(5) | 20(3) | 17(3) | 3(2) | 6(3) | 5(3) |
| C(27) | 21(5) | 28(3) | 22(3) | 0(3) | 1(3) | 3(3) |
| C(28) | 31(5) | 23(3) | 37(3) | 3(3) | 4(3) | 3(3) |
| C(29) | 26(5) | 21(4) | 40(3) | 0(3) | 8(4) | 3(3) |
| C(30) | 22(4) | 21(3) | 22(3) | 0(2) | 10(3) | 4(3) |
| C(31) | 26(6) | 28(4) | 54(4) | -7(3) | 16(4) | 2(3) |
| C(32) | 18(4) | 27(3) | 25(3) | -5(3) | 10(3) | -1(4) |
| C(33) | 30(5) | 17(3) | 31(3) | -1(2) | 11(3) | -4(3) |
| C(34) | 11(4) | 24(3) | 13(2) | 5(2) | 2(3) | 5(3) |
| C(35) | 23(5) | 19(3) | 10(3) | 4(2) | -1(3) | 6(3) |
| C(36) | 17(4) | 12(3) | 21(3) | -1(2) | 5(3) | 3(3) |
| C(37) | 23(5) | 29(3) | 24(3) | -5(3) | 11(3) | 5(3) |
| C(38) | 30(5) | 26(3) | 34(3) | -1(3) | 23(3) | 9(3) |
| C(39) | 18(4) | 27(3) | 21(3) | 1(3) | 3(3) | -4(3) |
| C(40) | 18(5) | 17(3) | 20(3) | 0(2) | 14(3) | 1(3) |
| N(1) | 56(3) | 32(2) | 67(2) | 4(1) | 29(2) | -2(2) |
| C(41) | 56(3) | 32(2) | 67(2) | 4(1) | 29(2) | -2(2) |
| C(42) | 56(3) | 32(2) | 67(2) | 4(1) | 29(2) | -2(2) |
| C(43) | 56(3) | 32(2) | 67(2) | 4(1) | 29(2) | -2(2) |
| C(44) | 56(3) | 32(2) | 67(2) | 4(1) | 29(2) | -2(2) |
| C(45) | 56(3) | 32(2) | 67(2) | 4(1) | 29(2) | -2(2) |

**Table S5.** Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$x $10^3$) for mo_IALVB88_0m_aa.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3) | 8373 | 5468 | 5104 | 24 |
| H(6) | 9757 | 5788 | 6210 | 43 |
| H(7) | 11697 | 5665 | 7143 | 56 |
| H(8) | 13553 | 5844 | 6868 | 55 |
| H(9) | 13594 | 6197 | 5699 | 53 |
| H(10) | 11657 | 6339 | 4770 | 34 |
| H(13) | 7945 | 5149 | 1589 | 18 |
| H(16) | 9829 | 4932 | 1467 | 25 |
| H(17) | 11754 | 4529 | 1560 | 34 |
| H(18) | 13478 | 4660 | 2638 | 27 |
| H(19) | 13093 | 5150 | 3673 | 27 |
| H(20) | 11147 | 5564 | 3589 | 24 |
| H(23) | 5834 | 7483 | 676 | 23 |
| H(26) | 3814 | 7447 | 392 | 25 |
| H(27) | 1741 | 7792 | 96 | 30 |
| H(28) | 1011 | 8297 | 976 | 38 |
| H(29) | 2371 | 8472 | 2171 | 36 |
| H(30) | 4392 | 8073 | 2503 | 25 |
| H(33) | 9136 | 8863 | 4097 | 31 |
| H(36) | 8206 | 9258 | 4858 | 20 |
| H(37) | 6840 | 9760 | 5403 | 29 |
| H(38) | 4810 | 9390 | 5250 | 33 |
| H(39) | 4078 | 8548 | 4465 | 27 |
| H(40) | 5425 | 8037 | 3942 | 20 |
| H(1A) | 4649 | 6672 | 3517 | 60 |
| H(41) | 4736 | 6305 | 2403 | 60 |
| H(42) | 2999 | 6278 | 1455 | 60 |
| H(43) | 1184 | 6579 | 1564 | 60 |
| H(44) | 979 | 6985 | 2549 | 60 |
| H(45) | 2576 | 7029 | 3689 | 60 |