**mo\_B1959\_0m**

|  |  |
| --- | --- |
| **Table 1 Crystal data and structure refinement for mo\_B1959\_0m.** | |
| Identification code | mo\_B1959\_0m |
| Empirical formula | C29H15Co4O14P |
| Formula weight | 854.10 |
| Temperature/K | 100.0 |
| Crystal system | monoclinic |
| Space group | P21/c |
| a/Å | 12.5987(10) |
| b/Å | 8.9773(9) |
| c/Å | 27.953(2) |
| α/° | 90 |
| β/° | 96.829(3) |
| γ/° | 90 |
| Volume/Å3 | 3139.2(5) |
| Z | 4 |
| ρcalcg/cm3 | 1.807 |
| μ/mm‑1 | 2.198 |
| F(000) | 1696.0 |
| Crystal size/mm3 | 0.377 × 0.194 × 0.15 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.768 to 66.294 |
| Index ranges | -19 ≤ h ≤ 19, -13 ≤ k ≤ 13, -42 ≤ l ≤ 39 |
| Reflections collected | 80869 |
| Independent reflections | 11959 [Rint = 0.0294, Rsigma = 0.0190] |
| Data/restraints/parameters | 11959/0/433 |
| Goodness-of-fit on F2 | 1.035 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0360, wR2 = 0.0957 |
| Final R indexes [all data] | R1 = 0.0421, wR2 = 0.1008 |
| Largest diff. peak/hole / e Å-3 | 3.32/-0.67 |

| **Table 2 Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement Parameters (Å2×103) for mo\_B1959\_0m. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.** | | | | |
| --- | --- | --- | --- | --- |
| **Atom** | ***x*** | ***y*** | ***z*** | **U(eq)** |
| Co1 | 6287.2(2) | 2350.8(3) | 3898.5(2) | 15.56(5) |
| Co2 | 5487.1(2) | 4855.3(3) | 3813.6(2) | 16.33(5) |
| Co3 | 5319.2(2) | 3145.7(3) | 3125.8(2) | 16.13(5) |
| Co4 | 4295.5(2) | 2610.6(3) | 3825.1(2) | 18.10(5) |
| P1 | 7971.4(4) | 2586.3(5) | 3846.9(2) | 16.38(8) |
| O1 | 8339.1(11) | 4236.0(15) | 4015.3(5) | 21.6(2) |
| O2 | 8347.9(11) | 2513.8(16) | 3319.1(5) | 21.3(3) |
| O3 | 8862.6(10) | 1528.2(16) | 4127.1(5) | 21.5(2) |
| O4 | 6032.9(14) | 39.1(17) | 3153.0(6) | 30.3(3) |
| O5 | 6093.3(14) | -153(2) | 4546.8(8) | 46.2(5) |
| O6 | 6633.5(12) | 4188.6(19) | 4767.1(5) | 26.8(3) |
| O7 | 6855.7(12) | 3886.9(18) | 2451.4(6) | 27.1(3) |
| O8 | 7064.0(13) | 7171.3(19) | 3680.4(6) | 32.6(3) |
| O9 | 4164.8(12) | 5972.3(16) | 2958.3(5) | 24.7(3) |
| O10 | 4053.5(14) | 6718(2) | 4305.0(6) | 32.0(3) |
| O11 | 2291.6(12) | 3928(2) | 3360.3(6) | 33.5(3) |
| O12 | 4099.4(14) | 2876(2) | 4867.9(6) | 31.7(3) |
| O13 | 3727.2(16) | -568(2) | 3662.3(7) | 39.4(4) |
| O14 | 3549.4(13) | 2131.2(18) | 2433.8(6) | 28.6(3) |
| C1 | 9350.6(14) | 4860(2) | 3985.9(7) | 21.0(3) |
| C2 | 9488.1(18) | 5751(3) | 3595.7(8) | 29.3(4) |
| C3 | 10468(2) | 6465(3) | 3589.7(11) | 39.1(5) |
| C4 | 11280.5(19) | 6277(3) | 3964.8(11) | 39.0(6) |
| C5 | 11128.0(17) | 5363(3) | 4348.7(10) | 35.5(5) |
| C6 | 10150.4(16) | 4643(2) | 4362.9(8) | 26.1(4) |
| C7 | 9069.5(14) | 1517(2) | 3148.0(6) | 19.7(3) |
| C8 | 10156.3(16) | 1678(2) | 3280.8(9) | 28.2(4) |
| C9 | 10855.0(17) | 729(3) | 3076.5(9) | 31.4(4) |
| C10 | 10473.9(19) | -341(3) | 2749.7(8) | 33.7(5) |
| C11 | 9383(2) | -485(4) | 2625.7(11) | 49.0(8) |
| C12 | 8670.1(19) | 450(3) | 2823.7(9) | 39.0(6) |
| C13 | 8685.3(13) | 574(2) | 4506.2(6) | 17.9(3) |
| C14 | 8654.4(15) | -938(2) | 4415.9(7) | 22.9(3) |
| C15 | 8499.8(17) | -1906(2) | 4789.5(8) | 27.6(4) |
| C16 | 8394.5(16) | -1360(2) | 5243.5(8) | 26.5(4) |
| C17 | 8442.6(18) | 165(3) | 5328.6(7) | 28.0(4) |
| C18 | 8589.0(17) | 1144(2) | 4957.8(7) | 25.3(4) |
| C19 | 5954.1(15) | 1211(2) | 3318.9(7) | 20.8(3) |
| C20 | 6226.0(15) | 816(3) | 4300.6(8) | 27.1(4) |
| C21 | 6310.4(14) | 3891(2) | 4373.1(6) | 19.7(3) |
| C22 | 6468.3(15) | 6266(2) | 3734.4(7) | 22.4(3) |
| C23 | 6267.1(15) | 3607(2) | 2712.5(7) | 20.8(3) |
| C24 | 4712.5(14) | 5121(2) | 3178.5(6) | 18.2(3) |
| C25 | 4615.8(16) | 5978(2) | 4125.9(7) | 23.3(3) |
| C26 | 3057.1(15) | 3438(2) | 3550.6(7) | 23.0(3) |
| C27 | 4170.5(15) | 2765(2) | 4469.6(8) | 24.2(3) |
| C28 | 3959.2(16) | 644(2) | 3720.3(8) | 26.2(4) |
| C29 | 4251.3(16) | 2500(2) | 2699.0(7) | 21.4(3) |

| **Table 3 Anisotropic Displacement Parameters (Å2×103) for mo\_B1959\_0m. The Anisotropic displacement factor exponent takes the form: -2π2[h2a\*2U11+2hka\*b\*U12+…].** | | | | | | |
| --- | --- | --- | --- | --- | --- | --- |
| **Atom** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| Co1 | 13.88(10) | 15.77(10) | 16.81(10) | 2.88(8) | 0.90(7) | 2.50(7) |
| Co2 | 17.21(10) | 16.0(1) | 15.39(10) | -0.28(7) | 0.37(8) | 2.12(8) |
| Co3 | 18.1(1) | 15.22(10) | 14.86(10) | 0.30(7) | 1.04(8) | 1.08(8) |
| Co4 | 15.29(10) | 19.80(11) | 19.15(11) | 3.04(8) | 1.80(8) | 0.91(8) |
| P1 | 14.77(17) | 17.12(19) | 17.20(18) | 1.82(14) | 1.77(14) | 2.55(14) |
| O1 | 17.5(5) | 18.8(6) | 29.2(7) | -2.0(5) | 5.1(5) | 0.0(4) |
| O2 | 21.0(6) | 25.6(7) | 17.7(6) | 2.3(5) | 3.9(5) | 6.8(5) |
| O3 | 16.3(5) | 26.2(7) | 22.1(6) | 8.1(5) | 2.3(4) | 4.9(5) |
| O4 | 41.1(9) | 19.4(6) | 29.7(7) | -1.9(5) | 0.8(6) | 7.0(6) |
| O5 | 23.6(7) | 49.4(11) | 65.1(13) | 38.8(10) | 3.3(8) | 2.6(7) |
| O6 | 26.2(7) | 36.7(8) | 16.6(6) | -1.8(5) | -1.5(5) | 7.2(6) |
| O7 | 28.8(7) | 27.7(7) | 25.9(7) | 0.7(6) | 7.5(5) | -1.8(6) |
| O8 | 30.9(8) | 25.4(7) | 38.7(9) | 2.7(6) | -7.6(6) | -6.4(6) |
| O9 | 29.5(7) | 21.7(6) | 21.8(6) | 2.3(5) | -1.1(5) | 5.5(5) |
| O10 | 37.5(8) | 34.9(8) | 24.4(7) | -1.9(6) | 7.3(6) | 15.1(7) |
| O11 | 21.4(7) | 38.9(9) | 38.8(9) | -0.7(7) | -2.7(6) | 5.9(6) |
| O12 | 33.3(8) | 36.9(8) | 25.1(7) | 1.5(6) | 4.8(6) | -3.9(7) |
| O13 | 47.7(10) | 26.3(8) | 42.8(10) | 3.1(7) | -0.7(8) | -4.8(7) |
| O14 | 30.5(7) | 26.5(7) | 27.1(7) | -2.9(6) | -4.0(6) | -5.1(6) |
| C1 | 17.5(7) | 18.1(7) | 27.5(8) | -3.5(6) | 3.7(6) | 0.4(6) |
| C2 | 28.7(9) | 25.7(9) | 34.3(10) | 4.5(8) | 6.7(8) | -0.7(7) |
| C3 | 36.2(12) | 27.7(11) | 56.7(15) | 3.2(10) | 19.8(11) | -5.2(9) |
| C4 | 24.6(9) | 26.8(10) | 67.3(17) | -14.6(11) | 13.4(10) | -6.6(8) |
| C5 | 21.5(9) | 33.1(11) | 50.3(14) | -17.4(10) | -1.9(9) | 0.9(8) |
| C6 | 23.5(8) | 26.1(9) | 27.9(9) | -6.9(7) | -0.1(7) | 2.6(7) |
| C7 | 18.9(7) | 22.8(8) | 17.8(7) | 2.2(6) | 4.3(6) | 4.1(6) |
| C8 | 19.0(8) | 25.2(9) | 41.4(11) | -3.8(8) | 7.4(7) | -1.4(7) |
| C9 | 19.8(8) | 30.1(10) | 46.2(12) | 1.5(9) | 11.8(8) | 1.6(7) |
| C10 | 33.8(11) | 40.3(12) | 28.0(10) | -1.4(9) | 7.7(8) | 15.6(9) |
| C11 | 39.6(13) | 62.0(18) | 41.7(14) | -30.6(13) | -9.6(11) | 18.7(13) |
| C12 | 26.6(10) | 52.7(15) | 35.0(11) | -20.2(11) | -7.9(8) | 11.1(10) |
| C13 | 13.9(6) | 20.1(7) | 19.1(7) | 2.7(6) | -0.7(5) | 2.7(5) |
| C14 | 22.0(8) | 21.6(8) | 24.7(8) | -3.1(6) | 0.4(6) | 2.2(6) |
| C15 | 26.4(9) | 18.5(8) | 37.4(11) | 3.4(7) | 1.2(8) | 1.7(7) |
| C16 | 22.1(8) | 28.5(9) | 28.5(9) | 10.1(7) | 1.2(7) | 1.4(7) |
| C17 | 34.2(10) | 30.6(10) | 19.3(8) | 1.3(7) | 3.7(7) | -1.8(8) |
| C18 | 31.9(9) | 20.7(8) | 23.8(8) | -1.8(7) | 5.4(7) | -1.0(7) |
| C19 | 22.0(8) | 17.8(7) | 22.5(8) | 0.8(6) | 2.4(6) | 1.7(6) |
| C20 | 16.1(7) | 30.2(10) | 34.3(10) | 12.4(8) | 0.9(7) | 4.0(7) |
| C21 | 16.7(7) | 24.9(8) | 17.6(7) | 2.1(6) | 2.3(5) | 3.6(6) |
| C22 | 22.8(8) | 21.2(8) | 21.9(8) | 0.6(6) | -2.6(6) | 2.4(6) |
| C23 | 21.6(7) | 17.7(7) | 22.5(8) | 0.8(6) | 0.4(6) | 0.6(6) |
| C24 | 20.7(7) | 17.3(7) | 16.8(7) | 0.1(5) | 2.6(6) | -0.7(6) |
| C25 | 25.2(8) | 26.2(9) | 17.6(7) | -0.3(6) | -1.1(6) | 5.3(7) |
| C26 | 20.5(7) | 23.8(8) | 24.7(8) | -0.4(7) | 2.5(6) | -0.2(6) |
| C27 | 18.6(7) | 27.7(9) | 26.6(9) | 6.1(7) | 3.4(6) | 0.6(7) |
| C28 | 24.4(8) | 27.6(9) | 26.7(9) | 6.7(7) | 2.6(7) | 1.0(7) |
| C29 | 25.3(8) | 17.9(7) | 20.6(8) | -1.1(6) | 0.9(6) | 0.8(6) |

| **Table 4 Bond Lengths for mo\_B1959\_0m.** | | | | | | |
| --- | --- | --- | --- | --- | --- | --- |
| **Atom** | **Atom** | **Length/Å** |  | **Atom** | **Atom** | **Length/Å** |
| Co1 | Co2 | 2.4639(4) |  | O5 | C20 | 1.134(3) |
| Co1 | Co3 | 2.4567(4) |  | O6 | C21 | 1.159(2) |
| Co1 | Co4 | 2.5042(4) |  | O7 | C23 | 1.129(2) |
| Co1 | P1 | 2.1542(5) |  | O8 | C22 | 1.128(3) |
| Co1 | C19 | 1.9199(19) |  | O9 | C24 | 1.157(2) |
| Co1 | C20 | 1.786(2) |  | O10 | C25 | 1.131(2) |
| Co1 | C21 | 1.9138(19) |  | O11 | C26 | 1.133(2) |
| Co2 | Co3 | 2.4494(4) |  | O12 | C27 | 1.132(3) |
| Co2 | Co4 | 2.5154(4) |  | O13 | C28 | 1.133(3) |
| Co2 | C21 | 1.9713(18) |  | O14 | C29 | 1.134(2) |
| Co2 | C22 | 1.802(2) |  | C1 | C2 | 1.380(3) |
| Co2 | C24 | 1.9360(18) |  | C1 | C6 | 1.383(3) |
| Co2 | C25 | 1.792(2) |  | C2 | C3 | 1.393(3) |
| Co3 | Co4 | 2.5129(4) |  | C3 | C4 | 1.385(4) |
| Co3 | C19 | 1.9608(19) |  | C4 | C5 | 1.383(4) |
| Co3 | C23 | 1.8057(19) |  | C5 | C6 | 1.396(3) |
| Co3 | C24 | 1.9433(18) |  | C7 | C8 | 1.383(3) |
| Co3 | C29 | 1.7854(19) |  | C7 | C12 | 1.373(3) |
| Co4 | C26 | 1.814(2) |  | C8 | C9 | 1.395(3) |
| Co4 | C27 | 1.832(2) |  | C9 | C10 | 1.372(4) |
| Co4 | C28 | 1.831(2) |  | C10 | C11 | 1.383(4) |
| P1 | O1 | 1.6054(15) |  | C11 | C12 | 1.392(3) |
| P1 | O2 | 1.6038(14) |  | C13 | C14 | 1.380(3) |
| P1 | O3 | 1.6022(14) |  | C13 | C18 | 1.381(3) |
| O1 | C1 | 1.403(2) |  | C14 | C15 | 1.390(3) |
| O2 | C7 | 1.400(2) |  | C15 | C16 | 1.382(3) |
| O3 | C13 | 1.401(2) |  | C16 | C17 | 1.390(3) |
| O4 | C19 | 1.159(2) |  | C17 | C18 | 1.388(3) |

| **Table 5 Bond Angles for mo\_B1959\_0m.** | | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Atom** | **Atom** | **Atom** | **Angle/˚** |  | **Atom** | **Atom** | **Atom** | **Angle/˚** |
| Co2 | Co1 | Co4 | 60.830(10) |  | Co1 | Co4 | Co3 | 58.636(10) |
| Co3 | Co1 | Co2 | 59.707(9) |  | Co3 | Co4 | Co2 | 58.303(10) |
| Co3 | Co1 | Co4 | 60.859(10) |  | C26 | Co4 | Co1 | 151.15(6) |
| P1 | Co1 | Co2 | 107.396(17) |  | C26 | Co4 | Co2 | 98.69(7) |
| P1 | Co1 | Co3 | 107.614(16) |  | C26 | Co4 | Co3 | 95.04(6) |
| P1 | Co1 | Co4 | 166.115(18) |  | C26 | Co4 | C27 | 102.40(9) |
| C19 | Co1 | Co2 | 111.05(6) |  | C26 | Co4 | C28 | 99.00(9) |
| C19 | Co1 | Co3 | 51.47(6) |  | C27 | Co4 | Co1 | 97.41(6) |
| C19 | Co1 | Co4 | 82.19(6) |  | C27 | Co4 | Co2 | 94.20(7) |
| C19 | Co1 | P1 | 96.55(6) |  | C27 | Co4 | Co3 | 149.60(6) |
| C20 | Co1 | Co2 | 135.80(7) |  | C28 | Co4 | Co1 | 97.69(7) |
| C20 | Co1 | Co3 | 136.34(7) |  | C28 | Co4 | Co2 | 153.83(7) |
| C20 | Co1 | Co4 | 90.32(6) |  | C28 | Co4 | Co3 | 100.97(7) |
| C20 | Co1 | P1 | 103.56(6) |  | C28 | Co4 | C27 | 100.64(9) |
| C20 | Co1 | C19 | 95.65(10) |  | O1 | P1 | Co1 | 108.85(5) |
| C20 | Co1 | C21 | 96.85(10) |  | O2 | P1 | Co1 | 117.32(6) |
| C21 | Co1 | Co2 | 51.68(5) |  | O2 | P1 | O1 | 101.57(8) |
| C21 | Co1 | Co3 | 111.39(5) |  | O3 | P1 | Co1 | 123.20(6) |
| C21 | Co1 | Co4 | 85.53(5) |  | O3 | P1 | O1 | 104.04(8) |
| C21 | Co1 | P1 | 92.38(6) |  | O3 | P1 | O2 | 99.15(7) |
| C21 | Co1 | C19 | 162.49(8) |  | C1 | O1 | P1 | 125.68(12) |
| Co1 | Co2 | Co4 | 60.377(11) |  | C7 | O2 | P1 | 127.99(12) |
| Co3 | Co2 | Co1 | 60.000(11) |  | C13 | O3 | P1 | 124.53(11) |
| Co3 | Co2 | Co4 | 60.798(11) |  | C2 | C1 | O1 | 118.54(18) |
| C21 | Co2 | Co1 | 49.61(6) |  | C2 | C1 | C6 | 122.38(19) |
| C21 | Co2 | Co3 | 109.61(6) |  | C6 | C1 | O1 | 118.93(18) |
| C21 | Co2 | Co4 | 84.06(6) |  | C1 | C2 | C3 | 118.1(2) |
| C22 | Co2 | Co1 | 111.99(6) |  | C4 | C3 | C2 | 120.7(2) |
| C22 | Co2 | Co3 | 109.91(6) |  | C5 | C4 | C3 | 120.1(2) |
| C22 | Co2 | Co4 | 169.73(6) |  | C4 | C5 | C6 | 120.1(2) |
| C22 | Co2 | C21 | 95.87(8) |  | C1 | C6 | C5 | 118.6(2) |
| C22 | Co2 | C24 | 94.55(8) |  | C8 | C7 | O2 | 120.28(18) |
| C24 | Co2 | Co1 | 110.89(5) |  | C12 | C7 | O2 | 118.02(17) |
| C24 | Co2 | Co3 | 50.98(5) |  | C12 | C7 | C8 | 121.56(19) |
| C24 | Co2 | Co4 | 82.75(5) |  | C7 | C8 | C9 | 118.6(2) |
| C24 | Co2 | C21 | 160.36(8) |  | C10 | C9 | C8 | 120.8(2) |
| C25 | Co2 | Co1 | 137.19(7) |  | C9 | C10 | C11 | 119.4(2) |
| C25 | Co2 | Co3 | 137.23(6) |  | C10 | C11 | C12 | 120.9(2) |
| C25 | Co2 | Co4 | 92.47(7) |  | C7 | C12 | C11 | 118.7(2) |
| C25 | Co2 | C21 | 98.95(8) |  | C14 | C13 | O3 | 117.82(17) |
| C25 | Co2 | C22 | 97.68(9) |  | C14 | C13 | C18 | 121.89(18) |
| C25 | Co2 | C24 | 96.10(8) |  | C18 | C13 | O3 | 120.24(17) |
| Co1 | Co3 | Co4 | 60.505(11) |  | C13 | C14 | C15 | 118.73(18) |
| Co2 | Co3 | Co1 | 60.293(11) |  | C16 | C15 | C14 | 120.39(19) |
| Co2 | Co3 | Co4 | 60.899(11) |  | C15 | C16 | C17 | 119.97(19) |
| C19 | Co3 | Co1 | 49.99(6) |  | C18 | C17 | C16 | 120.20(19) |
| C19 | Co3 | Co2 | 110.16(6) |  | C13 | C18 | C17 | 118.80(19) |
| C19 | Co3 | Co4 | 81.19(6) |  | Co1 | C19 | Co3 | 78.54(7) |
| C23 | Co3 | Co1 | 109.40(6) |  | O4 | C19 | Co1 | 143.23(16) |
| C23 | Co3 | Co2 | 110.89(6) |  | O4 | C19 | Co3 | 138.21(16) |
| C23 | Co3 | Co4 | 168.88(6) |  | O5 | C20 | Co1 | 174.04(18) |
| C23 | Co3 | C19 | 95.74(8) |  | Co1 | C21 | Co2 | 78.70(7) |
| C23 | Co3 | C24 | 97.78(8) |  | O6 | C21 | Co1 | 143.13(16) |
| C24 | Co3 | Co1 | 110.91(5) |  | O6 | C21 | Co2 | 138.13(16) |
| C24 | Co3 | Co2 | 50.72(5) |  | O8 | C22 | Co2 | 178.37(18) |
| C24 | Co3 | Co4 | 82.68(5) |  | O7 | C23 | Co3 | 179.42(19) |
| C24 | Co3 | C19 | 159.80(8) |  | Co2 | C24 | Co3 | 78.30(7) |
| C29 | Co3 | Co1 | 138.50(6) |  | O9 | C24 | Co2 | 140.62(15) |
| C29 | Co3 | Co2 | 135.71(6) |  | O9 | C24 | Co3 | 141.04(15) |
| C29 | Co3 | Co4 | 92.41(7) |  | O10 | C25 | Co2 | 177.05(18) |
| C29 | Co3 | C19 | 98.43(8) |  | O11 | C26 | Co4 | 176.96(19) |
| C29 | Co3 | C23 | 98.63(9) |  | O12 | C27 | Co4 | 179.2(2) |
| C29 | Co3 | C24 | 94.30(8) |  | O13 | C28 | Co4 | 178.1(2) |
| Co1 | Co4 | Co2 | 58.793(10) |  | O14 | C29 | Co3 | 177.40(19) |

| **Table 6 Torsion Angles for mo\_B1959\_0m.** | | | | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **A** | **B** | **C** | **D** | **Angle/˚** |  | **A** | **B** | **C** | **D** | **Angle/˚** |
| Co1 | P1 | O1 | C1 | -173.15(14) |  | O3 | C13 | C18 | C17 | -178.27(18) |
| Co1 | P1 | O2 | C7 | -121.19(15) |  | C1 | C2 | C3 | C4 | 0.2(4) |
| Co1 | P1 | O3 | C13 | -14.32(18) |  | C2 | C1 | C6 | C5 | 0.5(3) |
| P1 | O1 | C1 | C2 | 96.7(2) |  | C2 | C3 | C4 | C5 | 0.6(4) |
| P1 | O1 | C1 | C6 | -87.6(2) |  | C3 | C4 | C5 | C6 | -0.9(4) |
| P1 | O2 | C7 | C8 | -75.6(2) |  | C4 | C5 | C6 | C1 | 0.3(3) |
| P1 | O2 | C7 | C12 | 108.6(2) |  | C6 | C1 | C2 | C3 | -0.8(3) |
| P1 | O3 | C13 | C14 | 108.08(18) |  | C7 | C8 | C9 | C10 | 0.1(4) |
| P1 | O3 | C13 | C18 | -74.4(2) |  | C8 | C7 | C12 | C11 | -0.1(4) |
| O1 | P1 | O2 | C7 | 120.33(16) |  | C8 | C9 | C10 | C11 | -0.6(4) |
| O1 | P1 | O3 | C13 | 109.85(15) |  | C9 | C10 | C11 | C12 | 0.7(5) |
| O1 | C1 | C2 | C3 | 174.7(2) |  | C10 | C11 | C12 | C7 | -0.4(5) |
| O1 | C1 | C6 | C5 | -175.00(18) |  | C12 | C7 | C8 | C9 | 0.2(3) |
| O2 | P1 | O1 | C1 | -48.75(17) |  | C13 | C14 | C15 | C16 | -0.9(3) |
| O2 | P1 | O3 | C13 | -145.69(15) |  | C14 | C13 | C18 | C17 | -0.9(3) |
| O2 | C7 | C8 | C9 | -175.54(19) |  | C14 | C15 | C16 | C17 | 0.0(3) |
| O2 | C7 | C12 | C11 | 175.8(3) |  | C15 | C16 | C17 | C18 | 0.4(3) |
| O3 | P1 | O1 | C1 | 53.86(17) |  | C16 | C17 | C18 | C13 | 0.0(3) |
| O3 | P1 | O2 | C7 | 13.84(17) |  | C18 | C13 | C14 | C15 | 1.3(3) |
| O3 | C13 | C14 | C15 | 178.79(16) |  |  |  |  |  |  |

| **Table 7 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for mo\_B1959\_0m.** | | | | |
| --- | --- | --- | --- | --- |
| **Atom** | ***x*** | ***y*** | ***z*** | **U(eq)** |
| H2 | 8930.28 | 5874.27 | 3338.62 | 35 |
| H3 | 10581.06 | 7087.29 | 3325.48 | 47 |
| H4 | 11943.05 | 6777.68 | 3958.14 | 47 |
| H5 | 11689.57 | 5224.39 | 4603.27 | 43 |
| H6 | 10036.98 | 4016.39 | 4626.06 | 31 |
| H8 | 10421.65 | 2419.23 | 3506.42 | 34 |
| H9 | 11603.63 | 823.98 | 3164.76 | 38 |
| H10 | 10955.09 | -977.28 | 2609.96 | 40 |
| H11 | 9117.15 | -1232.43 | 2402.35 | 59 |
| H12 | 7921.43 | 351.9 | 2736.16 | 47 |
| H14 | 8737.33 | -1309.85 | 4104.31 | 28 |
| H15 | 8466.25 | -2948.88 | 4732.25 | 33 |
| H16 | 8289.2 | -2026.99 | 5497.49 | 32 |
| H17 | 8375.19 | 538.76 | 5641.51 | 34 |
| H18 | 8622.31 | 2187.79 | 5013.67 | 30 |

**Experimental**

Single crystals of C29H15Co4O14P **[mo\_B1959\_0m]** were **[]**. A suitable crystal was selected and **[]** on a **Bruker APEX-II CCD** diffractometer. The crystal was kept at 100.0 K during data collection. Using Olex2 [1], the structure was solved with the XT [2] structure solution program using Intrinsic Phasing and refined with the XL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

**Crystal structure determination of [mo\_B1959\_0m]**

**Crystal Data** for C29H15Co4O14P (*M*=854.10 g/mol): monoclinic, space group P21/c (no. 14), *a* = 12.5987(10) Å, *b* = 8.9773(9) Å, *c* = 27.953(2) Å, *β* = 96.829(3)°, *V*= 3139.2(5) Å3, *Z* = 4, *T* = 100.0 K, μ(MoKα) = 2.198 mm-1, *Dcalc* = 1.807 g/cm3, 80869 reflections measured (4.768° ≤ 2Θ ≤ 66.294°), 11959 unique (*R*int = 0.0294, Rsigma = 0.0190) which were used in all calculations. The final *R*1 was 0.0360 (I > 2σ(I)) and *wR*2 was 0.1008 (all data).

**Refinement model description**

Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso  
 At 1.2 times of:  
 All C(H) groups  
2.a Aromatic/amide H refined with riding coordinates:  
 C2(H2), C3(H3), C4(H4), C5(H5), C6(H6), C8(H8), C9(H9), C10(H10), C11(H11),  
 C12(H12), C14(H14), C15(H15), C16(H16), C17(H17), C18(H18)

This report has been created with Olex2, compiled on 2020.07.16 svn.r6f6c53a7 for OlexSys. Please [let us know](mailto:support@olex2.org?subject=Olex2%20Report) if there are any errors or if you would like to have additional features.