# phw1120

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| **Table 1 Crystal data and structure refinement for phw1120** | |
| Identification code | phw1120 |
| Empirical formula | C13H44.53486Cl1.46514O10.53486Ru2S6 |
| Formula weight | 816.02 |
| Temperature/K | 110.00(10) |
| Crystal system | monoclinic |
| Space group | P21/n |
| a/Å | 15.5134(6) |
| b/Å | 10.8600(4) |
| c/Å | 18.0560(12) |
| α/° | 90.00 |
| β/° | 106.470(6) |
| γ/° | 90.00 |
| Volume/Å3 | 2917.2(3) |
| Z | 4 |
| ρcalcmg/mm3 | 1.858 |
| m/mm‑1 | 1.643 |
| F(000) | 1663.0 |
| Crystal size/mm3 | 0.2844 × 0.1058 × 0.0886 |
| Radiation | Mo Kα (λ = 0.7107) |
| 2Θ range for data collection | 6.02 to 60.3° |
| Index ranges | -20 ≤ h ≤ 21, -14 ≤ k ≤ 14, -24 ≤ l ≤ 25 |
| Reflections collected | 21935 |
| Independent reflections | 7625[R(int) = 0.0379] |
| Data/restraints/parameters | 7625/1/355 |
| Goodness-of-fit on F2 | 1.181 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0420, wR2 = 0.0705 |
| Final R indexes [all data] | R1 = 0.0593, wR2 = 0.0767 |
| Largest diff. peak/hole / e Å-3 | 0.83/-0.90 |

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| **Table 2 Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement Parameters (Å2×103) for phw1120. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.** | | | | |
| **Atom** | ***x*** | ***y*** | ***z*** | **U(eq)** |
| C1 | 5058(3) | 5928(4) | 4051(3) | 25.4(10) |
| C2 | 6843(3) | 5958(4) | 4169(2) | 23.6(9) |
| C3 | 7611(3) | 2705(4) | 3728(3) | 29.4(10) |
| C4 | 7065(3) | 2566(4) | 2167(3) | 26.8(10) |
| C5 | 5683(3) | 5185(4) | 1334(2) | 19.7(8) |
| C6 | 4203(3) | 5737(4) | 1776(2) | 19.6(8) |
| C7 | 3526(3) | -100(4) | 4156(2) | 23.7(9) |
| C8 | 2998(3) | 2284(4) | 3938(3) | 24.5(9) |
| C9 | 2471(3) | 2496(4) | 1699(2) | 20.4(8) |
| C10 | 3098(3) | 409(4) | 1258(2) | 18.4(8) |
| C11 | 5391(3) | -473(4) | 2119(2) | 20.1(8) |
| C12 | 5760(3) | -710(4) | 3660(2) | 21.4(9) |
| Cl1 | 4102(14) | 3700(20) | 3056(15) | 22(2) |
| Cl2 | 5009(8) | 2345(10) | 1924(6) | 20.3(19) |
| O1 | 5660.5(18) | 2155(2) | 3598.1(16) | 11.9(5) |
| O2 | 4272(11) | 3528(17) | 3065(12) | 22(2) |
| O3 | 5073(7) | 2324(9) | 2184(3) | 16.8(18) |
| O4 | 6144(2) | 4149(3) | 4746.2(15) | 21.8(6) |
| O5 | 7514.3(18) | 4673(3) | 2874.5(17) | 22.4(6) |
| O6 | 5776.9(18) | 6609(2) | 2510.0(15) | 17.4(6) |
| O7 | 4652.0(19) | 1706(3) | 4700.3(15) | 20.0(6) |
| O8 | 2405.7(18) | 432(3) | 2415.3(17) | 21.7(6) |
| O9 | 4178.9(18) | -1317(2) | 2745.1(16) | 18.4(6) |
| Ru1 | 5575.82(19) | 3768.1(3) | 2960.13(16) | 9.92(7) |
| Ru2 | 4399.77(19) | 1612.2(3) | 2928.47(17) | 10.48(7) |
| S1 | 5943.1(7) | 4904.1(9) | 4036.8(5) | 15.81(19) |
| S2 | 6983.3(6) | 3568.4(8) | 2920.3(6) | 14.70(19) |
| S3 | 5361.8(6) | 5428.0(8) | 2187.7(5) | 12.13(18) |
| S4 | 3953.8(6) | 1350.6(9) | 3988.2(5) | 14.86(19) |
| S5 | 3044.9(6) | 1152.2(9) | 2118.3(5) | 13.41(18) |
| S6 | 4846.3(6) | -317.2(8) | 2855.9(5) | 12.65(18) |
| C13 | 5648(6) | 1421(7) | 34(4) | 83(3) |
| O10 | 5554(4) | 2689(5) | 9(3) | 86.8(17) |
| Cl3A | 3917.6(13) | 3083.5(17) | 484.1(9) | 30.5(5) |
| Cl3B | 7987(9) | -1052(11) | 4696(7) | 37(2) |
| O11A | 7938(7) | -570(7) | 4758(6) | 31.4(19) |
| O11B | 3591(13) | 3412(19) | 374(10) | 30.5(5) |

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| **Table 3 Anisotropic Displacement Parameters (Å2×103) for phw1120. The Anisotropic displacement factor exponent takes the form: -2π2[h2a\*2U11+...+2hka×b×U12]** | | | | | | |
| **Atom** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| C1 | 34(2) | 20(2) | 28(2) | -1.4(17) | 18(2) | 8.0(19) |
| C2 | 28(2) | 21(2) | 19(2) | -6.7(16) | 3.3(17) | -8.2(18) |
| C3 | 17(2) | 34(3) | 37(3) | 13(2) | 6.0(19) | 9(2) |
| C4 | 23(2) | 25(2) | 38(3) | -6.6(19) | 18(2) | 2.7(19) |
| C5 | 22(2) | 20(2) | 21(2) | 1.0(16) | 11.7(17) | -0.5(17) |
| C6 | 12.7(18) | 21(2) | 25(2) | 4.5(16) | 4.1(16) | 3.3(16) |
| C7 | 33(2) | 18(2) | 25(2) | -3.1(17) | 15.5(19) | -14.7(19) |
| C8 | 19(2) | 27(2) | 31(2) | -8.7(18) | 13.7(18) | 0.0(18) |
| C9 | 14.5(19) | 18.6(19) | 27(2) | 1.9(17) | 4.2(16) | 6.3(17) |
| C10 | 15.0(18) | 18.4(19) | 21(2) | -4.6(16) | 4.1(15) | -0.3(16) |
| C11 | 18(2) | 19(2) | 26(2) | -0.6(16) | 11.9(17) | 2.8(17) |
| C12 | 23(2) | 16.5(19) | 21(2) | 3.9(16) | 0.4(17) | 7.0(17) |
| Cl1 | 20(6) | 19(5) | 25.4(14) | 1(3) | 7(4) | -5(4) |
| Cl2 | 23(4) | 9(3) | 31(5) | 8(4) | 10(4) | 2(2) |
| O1 | 13.8(13) | 8.1(12) | 13.8(13) | 0.3(10) | 4.2(11) | -0.5(10) |
| O2 | 20(6) | 19(5) | 25.4(14) | 1(3) | 7(4) | -5(4) |
| O3 | 17(3) | 21(3) | 12(3) | 7(3) | 3(3) | 1.2(18) |
| O4 | 31.0(16) | 19.4(14) | 15.4(14) | 1.4(11) | 7.5(12) | -2.2(13) |
| O5 | 13.5(13) | 17.5(14) | 39.2(18) | 1.5(13) | 12.3(12) | -2.8(12) |
| O6 | 19.4(14) | 9.9(12) | 22.8(14) | -0.7(11) | 5.7(11) | -2.3(11) |
| O7 | 22.3(14) | 22.6(15) | 15.1(13) | -4.3(11) | 5.2(11) | -7.3(13) |
| O8 | 14.9(14) | 24.1(15) | 27.5(16) | 3.0(12) | 8.2(12) | -2.0(12) |
| O9 | 19.3(14) | 11.0(13) | 28.1(15) | -3.4(11) | 12.0(12) | -2.7(11) |
| Ru1 | 9.14(13) | 7.76(13) | 13.82(14) | -0.31(11) | 4.81(10) | -0.12(11) |
| Ru2 | 9.68(13) | 8.35(13) | 14.36(14) | -0.18(11) | 4.98(10) | -0.37(11) |
| S1 | 19.8(5) | 13.0(4) | 16.0(4) | -1.8(3) | 7.2(4) | -1.3(4) |
| S2 | 11.0(4) | 13.2(4) | 21.3(5) | 1.2(4) | 6.8(4) | 1.3(4) |
| S3 | 11.6(4) | 9.2(4) | 16.5(4) | 1.0(3) | 5.4(3) | 0.3(3) |
| S4 | 16.8(4) | 13.3(4) | 16.3(4) | -3.2(3) | 7.7(4) | -4.5(4) |
| S5 | 10.5(4) | 12.5(4) | 18.2(4) | 0.0(3) | 5.6(3) | 0.5(4) |
| S6 | 12.9(4) | 8.9(4) | 16.9(4) | -0.1(3) | 5.5(3) | 0.8(4) |
| C13 | 95(6) | 64(5) | 72(5) | -26(4) | -5(4) | 6(5) |
| O10 | 136(5) | 60(3) | 73(4) | 13(3) | 44(4) | 8(3) |
| Cl3A | 30.3(10) | 37.2(10) | 20.9(8) | 0.3(6) | 2.3(7) | -11.6(7) |
| Cl3B | 28(3) | 64(7) | 23(3) | -6(5) | 14(3) | -8(5) |
| O11A | 26(3) | 46(5) | 26(3) | -10(4) | 12(2) | -4(4) |
| O11B | 30.3(10) | 37.2(10) | 20.9(8) | 0.3(6) | 2.3(7) | -11.6(7) |

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| **Table 4 Bond Lengths for phw1120.** | | | | | | |
| **Atom** | **Atom** | **Length/Å** |  | **Atom** | **Atom** | **Length/Å** |
| C1 | S1 | 1.773(4) |  | O2 | Ru1 | 2.101(17) |
| C2 | S1 | 1.769(4) |  | O2 | Ru2 | 2.111(18) |
| C3 | S2 | 1.775(4) |  | O3 | Ru1 | 2.100(9) |
| C4 | S2 | 1.774(4) |  | O3 | Ru2 | 2.072(9) |
| C5 | S3 | 1.770(4) |  | O4 | S1 | 1.478(3) |
| C6 | S3 | 1.772(4) |  | O5 | S2 | 1.471(3) |
| C7 | S4 | 1.768(4) |  | O6 | S3 | 1.479(3) |
| C8 | S4 | 1.777(4) |  | O7 | S4 | 1.479(3) |
| C9 | S5 | 1.765(4) |  | O8 | S5 | 1.478(3) |
| C10 | S5 | 1.773(4) |  | O9 | S6 | 1.475(3) |
| C11 | S6 | 1.775(4) |  | Ru1 | Ru2 | 2.9588(4) |
| C12 | S6 | 1.769(4) |  | Ru1 | S1 | 2.2356(10) |
| Cl1 | Ru1 | 2.34(2) |  | Ru1 | S2 | 2.2156(10) |
| Cl1 | Ru2 | 2.34(2) |  | Ru1 | S3 | 2.2456(9) |
| Cl2 | Ru1 | 2.393(10) |  | Ru2 | S4 | 2.2297(10) |
| Cl2 | Ru2 | 2.406(11) |  | Ru2 | S5 | 2.2503(9) |
| O1 | Ru1 | 2.080(3) |  | Ru2 | S6 | 2.2223(9) |
| O1 | Ru2 | 2.072(3) |  | C13 | O10 | 1.384(8) |

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| **Table 5 Bond Angles for phw1120.** | | | | | | | | |
| **Atom** | **Atom** | **Atom** | **Angle/˚** |  | **Atom** | **Atom** | **Atom** | **Angle/˚** |
| Ru2 | Cl1 | Ru1 | 78.4(6) |  | O3 | Ru2 | Cl1 | 81.5(7) |
| Ru1 | Cl2 | Ru2 | 76.1(3) |  | O3 | Ru2 | Cl2 | 7.8(4) |
| Ru2 | O1 | Ru1 | 90.89(10) |  | O3 | Ru2 | O1 | 72.9(2) |
| Ru1 | O2 | Ru2 | 89.3(6) |  | O3 | Ru2 | O2 | 77.8(6) |
| Ru2 | O3 | Ru1 | 90.4(3) |  | O3 | Ru2 | Ru1 | 45.2(2) |
| Cl1 | Ru1 | Cl2 | 83.5(7) |  | O3 | Ru2 | S4 | 160.1(2) |
| Cl1 | Ru1 | Ru2 | 50.7(6) |  | O3 | Ru2 | S5 | 102.2(2) |
| Cl2 | Ru1 | Ru2 | 52.1(3) |  | O3 | Ru2 | S6 | 95.2(3) |
| O1 | Ru1 | Cl1 | 80.9(6) |  | S4 | Ru2 | Cl1 | 85.5(6) |
| O1 | Ru1 | Cl2 | 80.8(2) |  | S4 | Ru2 | Cl2 | 166.6(3) |
| O1 | Ru1 | O2 | 75.9(5) |  | S4 | Ru2 | Ru1 | 115.08(3) |
| O1 | Ru1 | O3 | 72.2(2) |  | S4 | Ru2 | S5 | 94.00(4) |
| O1 | Ru1 | Ru2 | 44.45(7) |  | S5 | Ru2 | Cl1 | 96.0(6) |
| O1 | Ru1 | S1 | 91.29(8) |  | S5 | Ru2 | Cl2 | 94.5(3) |
| O1 | Ru1 | S2 | 91.57(8) |  | S5 | Ru2 | Ru1 | 130.20(3) |
| O1 | Ru1 | S3 | 174.26(8) |  | S6 | Ru2 | Cl1 | 173.5(5) |
| O2 | Ru1 | Cl1 | 5.4(10) |  | S6 | Ru2 | Cl2 | 94.1(3) |
| O2 | Ru1 | Cl2 | 80.8(6) |  | S6 | Ru2 | Ru1 | 123.12(3) |
| O2 | Ru1 | Ru2 | 45.5(5) |  | S6 | Ru2 | S4 | 96.21(4) |
| O2 | Ru1 | S1 | 90.3(6) |  | S6 | Ru2 | S5 | 90.10(3) |
| O2 | Ru1 | S2 | 166.9(5) |  | C1 | S1 | Ru1 | 110.54(15) |
| O2 | Ru1 | S3 | 100.3(5) |  | C2 | S1 | C1 | 100.2(2) |
| O3 | Ru1 | Cl1 | 80.8(7) |  | C2 | S1 | Ru1 | 118.09(14) |
| O3 | Ru1 | Cl2 | 8.8(4) |  | O4 | S1 | C1 | 108.02(19) |
| O3 | Ru1 | O2 | 77.4(6) |  | O4 | S1 | C2 | 106.16(19) |
| O3 | Ru1 | Ru2 | 44.4(2) |  | O4 | S1 | Ru1 | 112.74(12) |
| O3 | Ru1 | S1 | 161.3(2) |  | C3 | S2 | Ru1 | 109.96(15) |
| O3 | Ru1 | S2 | 95.1(3) |  | C4 | S2 | C3 | 99.4(2) |
| O3 | Ru1 | S3 | 102.9(2) |  | C4 | S2 | Ru1 | 111.74(15) |
| S1 | Ru1 | Cl1 | 88.1(6) |  | O5 | S2 | C3 | 107.0(2) |
| S1 | Ru1 | Cl2 | 169.3(3) |  | O5 | S2 | C4 | 107.11(19) |
| S1 | Ru1 | Ru2 | 117.21(3) |  | O5 | S2 | Ru1 | 119.65(12) |
| S1 | Ru1 | S3 | 93.07(4) |  | C5 | S3 | C6 | 99.5(2) |
| S2 | Ru1 | Cl1 | 172.2(6) |  | C5 | S3 | Ru1 | 113.14(14) |
| S2 | Ru1 | Cl2 | 93.3(3) |  | C6 | S3 | Ru1 | 111.51(14) |
| S2 | Ru1 | Ru2 | 122.00(3) |  | O6 | S3 | C5 | 105.86(18) |
| S2 | Ru1 | S1 | 94.11(4) |  | O6 | S3 | C6 | 106.11(18) |
| S2 | Ru1 | S3 | 91.83(3) |  | O6 | S3 | Ru1 | 118.74(11) |
| S3 | Ru1 | Cl1 | 95.5(6) |  | C7 | S4 | C8 | 99.7(2) |
| S3 | Ru1 | Cl2 | 94.4(2) |  | C7 | S4 | Ru2 | 118.86(14) |
| S3 | Ru1 | Ru2 | 129.90(3) |  | C8 | S4 | Ru2 | 109.96(15) |
| Cl1 | Ru2 | Cl2 | 83.3(7) |  | O7 | S4 | C7 | 107.57(19) |
| Cl1 | Ru2 | Ru1 | 50.9(5) |  | O7 | S4 | C8 | 106.85(18) |
| Cl2 | Ru2 | Ru1 | 51.7(3) |  | O7 | S4 | Ru2 | 112.58(12) |
| O1 | Ru2 | Cl1 | 81.2(6) |  | C9 | S5 | C10 | 98.24(19) |
| O1 | Ru2 | Cl2 | 80.7(3) |  | C9 | S5 | Ru2 | 111.09(14) |
| O1 | Ru2 | O2 | 75.9(5) |  | C10 | S5 | Ru2 | 113.81(13) |
| O1 | Ru2 | Ru1 | 44.66(7) |  | O8 | S5 | C9 | 106.55(18) |
| O1 | Ru2 | S4 | 90.38(8) |  | O8 | S5 | C10 | 106.24(18) |
| O1 | Ru2 | S5 | 174.62(8) |  | O8 | S5 | Ru2 | 118.73(12) |
| O1 | Ru2 | S6 | 92.54(8) |  | C11 | S6 | Ru2 | 110.90(14) |
| O2 | Ru2 | Cl1 | 5.8(10) |  | C12 | S6 | C11 | 98.7(2) |
| O2 | Ru2 | Cl2 | 80.3(6) |  | C12 | S6 | Ru2 | 111.69(14) |
| O2 | Ru2 | Ru1 | 45.2(5) |  | O9 | S6 | C11 | 107.03(18) |
| O2 | Ru2 | S4 | 87.9(6) |  | O9 | S6 | C12 | 107.58(18) |
| O2 | Ru2 | S5 | 101.1(5) |  | O9 | S6 | Ru2 | 118.94(12) |
| O2 | Ru2 | S6 | 167.8(5) |  |  |  |  |  |

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| **Table 6 Hydrogen Bonds for phw1120.** | | | | | | |
| **D** | **H** | **A** | **d(D-H)/Å** | **d(H-A)/Å** | **d(D-A)/Å** | **D-H-A/°** |
| C1 | H1C | Cl1 | 0.98 | 2.51 | 3.12(2) | 120.9 |
| C2 | H2C | O6 | 0.98 | 2.26 | 3.065(5) | 138.5 |
| C6 | H6C | O81 | 0.98 | 2.42 | 3.246(5) | 141.7 |
| C7 | H7A | O8 | 0.98 | 2.40 | 3.183(5) | 136.5 |
| C9 | H9A | O91 | 0.98 | 2.57 | 3.267(5) | 128.3 |
| C11 | H11B | O62 | 0.98 | 2.37 | 3.264(5) | 151.7 |
| C11 | H11C | O53 | 0.98 | 2.47 | 3.251(5) | 136.6 |
| O1 | H1 | O4 | 0.72(6) | 2.42(6) | 2.944(4) | 131(6) |
| O1 | H1 | O7 | 0.72(6) | 2.37(6) | 2.900(4) | 132(6) |
| O2 | H2 | O81 | 0.95(7) | 2.43(7) | 3.244(16) | 144(6) |
| O3 | H3 | Cl3A | 0.90(8) | 2.32(8) | 3.193(7) | 164(7) |
| O10 | H10 | Cl3A | 0.84 | 2.11 | 2.932(6) | 167.2 |
| O11A | H11D | O103 | 0.87 | 2.08 | 2.944(11) | 173.8 |
| O11A | H11E | Cl3A4 | 0.87 | 2.35 | 3.193(8) | 163.6 |
| O11A | H11E | O11B4 | 0.87 | 1.83 | 2.67(2) | 161.1 |
| O11B | H11F | Cl3B5 | 0.98 | 2.23 | 3.15(2) | 156.1 |
| O11B | H11F | O11A5 | 0.98 | 1.76 | 2.67(2) | 151.1 |
| O11B | H11G | Cl2 | 0.98 | 2.31 | 3.24(2) | 159.4 |

11/2-X,1/2+Y,1/2-Z; 2+X,-1+Y,+Z; 33/2-X,-1/2+Y,1/2-Z; 41/2+X,1/2-Y,1/2+Z; 5-1/2+X,1/2-Y,-1/2+Z

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| **Table 7 Torsion Angles for phw1120.** | | | | | | | | | | |
| **A** | **B** | **C** | **D** | **Angle/˚** |  | **A** | **B** | **C** | **D** | **Angle/˚** |
| Cl1 | Ru1 | Ru2 | Cl2 | 116.8(9) |  | Ru1 | O1 | Ru2 | O3 | 42.5(3) |
| Cl1 | Ru1 | Ru2 | O1 | -122.9(8) |  | Ru1 | O1 | Ru2 | S4 | -126.61(8) |
| Cl1 | Ru1 | Ru2 | O2 | -1.9(16) |  | Ru1 | O1 | Ru2 | S6 | 137.16(8) |
| Cl1 | Ru1 | Ru2 | O3 | 122.6(9) |  | Ru1 | O2 | Ru2 | Cl1 | -165(12) |
| Cl1 | Ru1 | Ru2 | S4 | -60.4(8) |  | Ru1 | O2 | Ru2 | Cl2 | -44.3(6) |
| Cl1 | Ru1 | Ru2 | S5 | 59.3(8) |  | Ru1 | O2 | Ru2 | O1 | 38.4(5) |
| Cl1 | Ru1 | Ru2 | S6 | -177.1(8) |  | Ru1 | O2 | Ru2 | O3 | -36.8(5) |
| Cl1 | Ru1 | S1 | C1 | -37.1(6) |  | Ru1 | O2 | Ru2 | S4 | 129.3(6) |
| Cl1 | Ru1 | S1 | C2 | -151.7(6) |  | Ru1 | O2 | Ru2 | S5 | -137.0(5) |
| Cl1 | Ru1 | S1 | O4 | 83.9(6) |  | Ru1 | O2 | Ru2 | S6 | 19(3) |
| Cl1 | Ru1 | S3 | C5 | -126.5(6) |  | Ru1 | O3 | Ru2 | Cl1 | 41.3(6) |
| Cl1 | Ru1 | S3 | C6 | -15.3(6) |  | Ru1 | O3 | Ru2 | Cl2 | 145(4) |
| Cl1 | Ru1 | S3 | O6 | 108.5(6) |  | Ru1 | O3 | Ru2 | O1 | -42.0(2) |
| Cl1 | Ru2 | S4 | C7 | 155.0(6) |  | Ru1 | O3 | Ru2 | O2 | 36.8(6) |
| Cl1 | Ru2 | S4 | C8 | 41.1(6) |  | Ru1 | O3 | Ru2 | S4 | -8.1(10) |
| Cl1 | Ru2 | S4 | O7 | -77.9(6) |  | Ru1 | O3 | Ru2 | S5 | 135.7(2) |
| Cl1 | Ru2 | S5 | C9 | 17.0(6) |  | Ru1 | O3 | Ru2 | S6 | -133.0(3) |
| Cl1 | Ru2 | S5 | C10 | 126.8(6) |  | Ru1 | Ru2 | S4 | C7 | -162.42(18) |
| Cl1 | Ru2 | S5 | O8 | -107.0(6) |  | Ru1 | Ru2 | S4 | C8 | 83.65(15) |
| Cl2 | Ru1 | Ru2 | Cl1 | -116.8(9) |  | Ru1 | Ru2 | S4 | O7 | -35.36(14) |
| Cl2 | Ru1 | Ru2 | O1 | 120.3(4) |  | Ru1 | Ru2 | S5 | C9 | -25.12(16) |
| Cl2 | Ru1 | Ru2 | O2 | -118.7(9) |  | Ru1 | Ru2 | S5 | C10 | 84.65(15) |
| Cl2 | Ru1 | Ru2 | O3 | 5.8(7) |  | Ru1 | Ru2 | S5 | O8 | -149.15(13) |
| Cl2 | Ru1 | Ru2 | S4 | -177.3(3) |  | Ru1 | Ru2 | S6 | C11 | -47.68(15) |
| Cl2 | Ru1 | Ru2 | S5 | -57.5(3) |  | Ru1 | Ru2 | S6 | C12 | 61.34(16) |
| Cl2 | Ru1 | Ru2 | S6 | 66.1(3) |  | Ru1 | Ru2 | S6 | O9 | -172.40(13) |
| Cl2 | Ru1 | S1 | C1 | -75.6(15) |  | Ru2 | Cl1 | Ru1 | Cl2 | 45.1(5) |
| Cl2 | Ru1 | S1 | C2 | 169.8(15) |  | Ru2 | Cl1 | Ru1 | O1 | -36.6(4) |
| Cl2 | Ru1 | S1 | O4 | 45.4(15) |  | Ru2 | Cl1 | Ru1 | O2 | -14(12) |
| Cl2 | Ru1 | S2 | C3 | -107.1(3) |  | Ru2 | Cl1 | Ru1 | O3 | 36.7(5) |
| Cl2 | Ru1 | S2 | C4 | 2.4(3) |  | Ru2 | Cl1 | Ru1 | S1 | -128.2(5) |
| Cl2 | Ru1 | S2 | O5 | 128.6(3) |  | Ru2 | Cl1 | Ru1 | S3 | 138.9(5) |
| Cl2 | Ru1 | S3 | C5 | -42.6(3) |  | Ru2 | Cl2 | Ru1 | Cl1 | -44.0(6) |
| Cl2 | Ru1 | S3 | C6 | 68.7(3) |  | Ru2 | Cl2 | Ru1 | O1 | 37.77(19) |
| Cl2 | Ru1 | S3 | O6 | -167.5(3) |  | Ru2 | Cl2 | Ru1 | O2 | -39.3(6) |
| Cl2 | Ru2 | S4 | C7 | -171.7(12) |  | Ru2 | Cl2 | Ru1 | O3 | 27(3) |
| Cl2 | Ru2 | S4 | C8 | 74.4(12) |  | Ru2 | Cl2 | Ru1 | S1 | -5.3(16) |
| Cl2 | Ru2 | S4 | O7 | -44.6(12) |  | Ru2 | Cl2 | Ru1 | S2 | 128.8(2) |
| Cl2 | Ru2 | S5 | C9 | -66.8(3) |  | Ru2 | Cl2 | Ru1 | S3 | -139.08(19) |
| Cl2 | Ru2 | S5 | C10 | 43.0(3) |  | Ru2 | O1 | Ru1 | Cl1 | 41.2(6) |
| Cl2 | Ru2 | S5 | O8 | 169.2(3) |  | Ru2 | O1 | Ru1 | Cl2 | -43.7(3) |
| Cl2 | Ru2 | S6 | C11 | -1.6(3) |  | Ru2 | O1 | Ru1 | O2 | 39.1(6) |
| Cl2 | Ru2 | S6 | C12 | 107.4(3) |  | Ru2 | O1 | Ru1 | O3 | -42.0(3) |
| Cl2 | Ru2 | S6 | O9 | -126.4(3) |  | Ru2 | O1 | Ru1 | S1 | 129.05(8) |
| O1 | Ru1 | Ru2 | Cl1 | 122.9(8) |  | Ru2 | O1 | Ru1 | S2 | -136.80(8) |
| O1 | Ru1 | Ru2 | Cl2 | -120.3(4) |  | Ru2 | O2 | Ru1 | Cl1 | 164(13) |
| O1 | Ru1 | Ru2 | O2 | 121.0(8) |  | Ru2 | O2 | Ru1 | Cl2 | 44.5(6) |
| O1 | Ru1 | Ru2 | O3 | -114.5(4) |  | Ru2 | O2 | Ru1 | O1 | -38.2(5) |
| O1 | Ru1 | Ru2 | S4 | 62.41(11) |  | Ru2 | O2 | Ru1 | O3 | 36.3(5) |
| O1 | Ru1 | Ru2 | S5 | -177.84(12) |  | Ru2 | O2 | Ru1 | S1 | -129.5(6) |
| O1 | Ru1 | Ru2 | S6 | -54.21(11) |  | Ru2 | O2 | Ru1 | S2 | -20(3) |
| O1 | Ru1 | S1 | C1 | -118.02(17) |  | Ru2 | O2 | Ru1 | S3 | 137.3(5) |
| O1 | Ru1 | S1 | C2 | 127.45(19) |  | Ru2 | O3 | Ru1 | Cl1 | -41.4(6) |
| O1 | Ru1 | S1 | O4 | 2.99(16) |  | Ru2 | O3 | Ru1 | Cl2 | -149(4) |
| O1 | Ru1 | S2 | C3 | -26.17(19) |  | Ru2 | O3 | Ru1 | O1 | 42.0(2) |
| O1 | Ru1 | S2 | C4 | 83.26(19) |  | Ru2 | O3 | Ru1 | O2 | -37.0(6) |
| O1 | Ru1 | S2 | O5 | -150.49(17) |  | Ru2 | O3 | Ru1 | S1 | 13.0(11) |
| O1 | Ru2 | S4 | C7 | -123.9(2) |  | Ru2 | O3 | Ru1 | S2 | 132.0(3) |
| O1 | Ru2 | S4 | C8 | 122.18(17) |  | Ru2 | O3 | Ru1 | S3 | -134.9(2) |
| O1 | Ru2 | S4 | O7 | 3.17(15) |  | Ru2 | Ru1 | S1 | C1 | -80.33(16) |
| O1 | Ru2 | S6 | C11 | -82.48(17) |  | Ru2 | Ru1 | S1 | C2 | 165.15(17) |
| O1 | Ru2 | S6 | C12 | 26.54(18) |  | Ru2 | Ru1 | S1 | O4 | 40.69(14) |
| O1 | Ru2 | S6 | O9 | 152.80(15) |  | Ru2 | Ru1 | S2 | C3 | -60.59(18) |
| O2 | Ru1 | Ru2 | Cl1 | 1.9(16) |  | Ru2 | Ru1 | S2 | C4 | 48.83(17) |
| O2 | Ru1 | Ru2 | Cl2 | 118.7(9) |  | Ru2 | Ru1 | S2 | O5 | 175.09(14) |
| O2 | Ru1 | Ru2 | O1 | -121.0(8) |  | Ru2 | Ru1 | S3 | C5 | -84.94(15) |
| O2 | Ru1 | Ru2 | O3 | 124.5(9) |  | Ru2 | Ru1 | S3 | C6 | 26.28(16) |
| O2 | Ru1 | Ru2 | S4 | -58.6(8) |  | Ru2 | Ru1 | S3 | O6 | 150.08(13) |
| O2 | Ru1 | Ru2 | S5 | 61.2(8) |  | S1 | Ru1 | Ru2 | Cl1 | 62.1(8) |
| O2 | Ru1 | Ru2 | S6 | -175.2(8) |  | S1 | Ru1 | Ru2 | Cl2 | 178.9(3) |
| O2 | Ru1 | S1 | C1 | -42.1(5) |  | S1 | Ru1 | Ru2 | O1 | -60.80(11) |
| O2 | Ru1 | S1 | C2 | -156.6(5) |  | S1 | Ru1 | Ru2 | O2 | 60.2(8) |
| O2 | Ru1 | S1 | O4 | 78.9(5) |  | S1 | Ru1 | Ru2 | O3 | -175.3(4) |
| O2 | Ru1 | S2 | C3 | -44(3) |  | S1 | Ru1 | Ru2 | S4 | 1.61(4) |
| O2 | Ru1 | S2 | C4 | 65(3) |  | S1 | Ru1 | Ru2 | S5 | 121.36(4) |
| O2 | Ru1 | S2 | O5 | -168(3) |  | S1 | Ru1 | Ru2 | S6 | -115.01(4) |
| O2 | Ru1 | S3 | C5 | -124.0(6) |  | S1 | Ru1 | S2 | C3 | 65.24(18) |
| O2 | Ru1 | S3 | C6 | -12.8(6) |  | S1 | Ru1 | S2 | C4 | 174.67(17) |
| O2 | Ru1 | S3 | O6 | 111.0(6) |  | S1 | Ru1 | S2 | O5 | -59.08(15) |
| O2 | Ru2 | S4 | C7 | 160.3(5) |  | S1 | Ru1 | S3 | C5 | 145.15(15) |
| O2 | Ru2 | S4 | C8 | 46.3(5) |  | S1 | Ru1 | S3 | C6 | -103.63(16) |
| O2 | Ru2 | S4 | O7 | -72.7(5) |  | S1 | Ru1 | S3 | O6 | 20.17(13) |
| O2 | Ru2 | S5 | C9 | 14.2(6) |  | S2 | Ru1 | Ru2 | Cl1 | 176.7(8) |
| O2 | Ru2 | S5 | C10 | 124.0(6) |  | S2 | Ru1 | Ru2 | Cl2 | -66.5(3) |
| O2 | Ru2 | S5 | O8 | -109.8(6) |  | S2 | Ru1 | Ru2 | O1 | 53.80(11) |
| O2 | Ru2 | S6 | C11 | -64(3) |  | S2 | Ru1 | Ru2 | O2 | 174.8(8) |
| O2 | Ru2 | S6 | C12 | 45(3) |  | S2 | Ru1 | Ru2 | O3 | -60.7(4) |
| O2 | Ru2 | S6 | O9 | 171(3) |  | S2 | Ru1 | Ru2 | S4 | 116.21(4) |
| O3 | Ru1 | Ru2 | Cl1 | -122.6(9) |  | S2 | Ru1 | Ru2 | S5 | -124.04(5) |
| O3 | Ru1 | Ru2 | Cl2 | -5.8(7) |  | S2 | Ru1 | Ru2 | S6 | -0.41(5) |
| O3 | Ru1 | Ru2 | O1 | 114.5(4) |  | S2 | Ru1 | S1 | C1 | 150.30(16) |
| O3 | Ru1 | Ru2 | O2 | -124.5(9) |  | S2 | Ru1 | S1 | C2 | 35.78(17) |
| O3 | Ru1 | Ru2 | S4 | 177.0(4) |  | S2 | Ru1 | S1 | O4 | -88.68(14) |
| O3 | Ru1 | Ru2 | S5 | -63.3(4) |  | S2 | Ru1 | S3 | C5 | 50.93(15) |
| O3 | Ru1 | Ru2 | S6 | 60.3(4) |  | S2 | Ru1 | S3 | C6 | 162.15(15) |
| O3 | Ru1 | S1 | C1 | -90.5(9) |  | S2 | Ru1 | S3 | O6 | -74.05(13) |
| O3 | Ru1 | S1 | C2 | 155.0(9) |  | S3 | Ru1 | Ru2 | Cl1 | -58.5(8) |
| O3 | Ru1 | S1 | O4 | 30.5(9) |  | S3 | Ru1 | Ru2 | Cl2 | 58.4(3) |
| O3 | Ru1 | S2 | C3 | -98.4(3) |  | S3 | Ru1 | Ru2 | O1 | 178.65(12) |
| O3 | Ru1 | S2 | C4 | 11.0(3) |  | S3 | Ru1 | Ru2 | O2 | -60.4(8) |
| O3 | Ru1 | S2 | O5 | 137.3(2) |  | S3 | Ru1 | Ru2 | O3 | 64.1(4) |
| O3 | Ru1 | S3 | C5 | -44.7(3) |  | S3 | Ru1 | Ru2 | S4 | -118.94(4) |
| O3 | Ru1 | S3 | C6 | 66.5(3) |  | S3 | Ru1 | Ru2 | S5 | 0.81(5) |
| O3 | Ru1 | S3 | O6 | -169.7(3) |  | S3 | Ru1 | Ru2 | S6 | 124.45(4) |
| O3 | Ru2 | S4 | C7 | -156.0(8) |  | S3 | Ru1 | S1 | C1 | 58.25(16) |
| O3 | Ru2 | S4 | C8 | 90.0(8) |  | S3 | Ru1 | S1 | C2 | -56.28(17) |
| O3 | Ru2 | S4 | O7 | -29.0(8) |  | S3 | Ru1 | S1 | O4 | 179.26(14) |
| O3 | Ru2 | S5 | C9 | -65.6(3) |  | S3 | Ru1 | S2 | C3 | 158.45(18) |
| O3 | Ru2 | S5 | C10 | 44.2(3) |  | S3 | Ru1 | S2 | C4 | -92.13(17) |
| O3 | Ru2 | S5 | O8 | 170.4(3) |  | S3 | Ru1 | S2 | O5 | 34.13(15) |
| O3 | Ru2 | S6 | C11 | -9.4(3) |  | S4 | Ru2 | S5 | C9 | 102.86(16) |
| O3 | Ru2 | S6 | C12 | 99.6(3) |  | S4 | Ru2 | S5 | C10 | -147.37(15) |
| O3 | Ru2 | S6 | O9 | -134.1(3) |  | S4 | Ru2 | S5 | O8 | -21.17(14) |
| Ru1 | Cl1 | Ru2 | Cl2 | -44.9(5) |  | S4 | Ru2 | S6 | C11 | -173.14(15) |
| Ru1 | Cl1 | Ru2 | O1 | 36.7(4) |  | S4 | Ru2 | S6 | C12 | -64.12(16) |
| Ru1 | Cl1 | Ru2 | O2 | 13(11) |  | S4 | Ru2 | S6 | O9 | 62.14(14) |
| Ru1 | Cl1 | Ru2 | O3 | -37.2(5) |  | S5 | Ru2 | S4 | C7 | 59.25(18) |
| Ru1 | Cl1 | Ru2 | S4 | 127.8(5) |  | S5 | Ru2 | S4 | C8 | -54.68(15) |
| Ru1 | Cl1 | Ru2 | S5 | -138.7(4) |  | S5 | Ru2 | S4 | O7 | -173.70(13) |
| Ru1 | Cl2 | Ru2 | Cl1 | 44.2(6) |  | S5 | Ru2 | S6 | C11 | 92.83(15) |
| Ru1 | Cl2 | Ru2 | O1 | -37.9(2) |  | S5 | Ru2 | S6 | C12 | -158.15(16) |
| Ru1 | Cl2 | Ru2 | O2 | 39.2(5) |  | S5 | Ru2 | S6 | O9 | -31.89(14) |
| Ru1 | Cl2 | Ru2 | O3 | -32(4) |  | S6 | Ru2 | S4 | C7 | -31.28(18) |
| Ru1 | Cl2 | Ru2 | S4 | 10.7(14) |  | S6 | Ru2 | S4 | C8 | -145.21(15) |
| Ru1 | Cl2 | Ru2 | S5 | 139.7(2) |  | S6 | Ru2 | S4 | O7 | 95.77(13) |
| Ru1 | Cl2 | Ru2 | S6 | -129.9(2) |  | S6 | Ru2 | S5 | C9 | -160.91(15) |
| Ru1 | O1 | Ru2 | Cl1 | -41.2(6) |  | S6 | Ru2 | S5 | C10 | -51.14(15) |
| Ru1 | O1 | Ru2 | Cl2 | 43.4(3) |  | S6 | Ru2 | S5 | O8 | 75.06(14) |
| Ru1 | O1 | Ru2 | O2 | -38.9(6) |  |  |  |  |  |  |

|  |  |  |  |  |
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| **Table 8 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for phw1120.** | | | | |
| **Atom** | ***x*** | ***y*** | ***z*** | **U(eq)** |
| H1A | 4973 | 6520 | 3626 | 38 |
| H1B | 5209 | 6370 | 4544 | 38 |
| H1C | 4502 | 5459 | 3990 | 38 |
| H2A | 7410 | 5504 | 4259 | 35 |
| H2B | 6868 | 6485 | 4615 | 35 |
| H2C | 6751 | 6469 | 3705 | 35 |
| H3A | 7622 | 3143 | 4205 | 44 |
| H3B | 8228 | 2598 | 3698 | 44 |
| H3C | 7331 | 1895 | 3728 | 44 |
| H4A | 6707 | 1825 | 2172 | 40 |
| H4B | 7695 | 2335 | 2244 | 40 |
| H4C | 6839 | 2986 | 1669 | 40 |
| H5A | 6337 | 5088 | 1465 | 30 |
| H5B | 5500 | 5894 | 989 | 30 |
| H5C | 5391 | 4439 | 1074 | 30 |
| H6A | 3913 | 5022 | 1476 | 29 |
| H6B | 4133 | 6456 | 1436 | 29 |
| H6C | 3922 | 5904 | 2188 | 29 |
| H7A | 3061 | -362 | 3692 | 35 |
| H7B | 3267 | -37 | 4590 | 35 |
| H7C | 4015 | -706 | 4278 | 35 |
| H8A | 3161 | 3153 | 3921 | 37 |
| H8B | 2790 | 2136 | 4395 | 37 |
| H8C | 2518 | 2077 | 3472 | 37 |
| H9A | 2349 | 3012 | 2103 | 31 |
| H9B | 1902 | 2268 | 1324 | 31 |
| H9C | 2843 | 2955 | 1437 | 31 |
| H10A | 3487 | 883 | 1020 | 28 |
| H10B | 2493 | 356 | 898 | 28 |
| H10C | 3344 | -421 | 1380 | 28 |
| H11A | 5007 | -131 | 1636 | 30 |
| H11B | 5502 | -1347 | 2046 | 30 |
| H11C | 5964 | -29 | 2269 | 30 |
| H12A | 6210 | -52 | 3755 | 32 |
| H12B | 6031 | -1481 | 3553 | 32 |
| H12C | 5545 | -815 | 4116 | 32 |
| H1 | 5630(40) | 2330(60) | 3980(30) | 60(20) |
| H2 | 3770(50) | 3910(70) | 2710(40) | 40(20) |
| H3 | 4720(50) | 2670(70) | 1750(40) | 40(30) |
| H13A | 5894 | 1155 | 572 | 124 |
| H13B | 6058 | 1173 | -264 | 124 |
| H13C | 5060 | 1036 | -187 | 124 |
| H10 | 5061 | 2880 | 85 | 130 |
| H11D | 8366 | -1103 | 4791 | 47 |
| H11E | 8168 | 163 | 4857 | 47 |
| H11F | 3434 | 4291 | 322 | 46 |
| H11G | 3944 | 3237 | 907 | 46 |

Experimental

Single crystals of C13H44.53486Cl1.46514O10.53486Ru2S6 [phw1120] were [?]. A suitable crystal was selected and [oil on loop] on a Oxford Diffraction SuperNova diffractometer. The crystal was kept at 110.00(10) K during data collection. Using Olex2 [1], the structure was solved with the XS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. (2009). 42, 339-341.
2. SHELX, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122
3. SHELX, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122

Crystal structure determination of **[phw1120]**

**Crystal Data** for C13H44.53486Cl1.46514O10.53486Ru2S6 (*M*=816.02): monoclinic, space group P21/n (no. 14), *a* = 15.5134(6) Å, *b* = 10.8600(4) Å, *c* = 18.0560(12) Å, *β* = 106.470(6)°, *V*= 2917.2(3) Å3, *Z* = 4, *T* = 110.00(10) K, μ(Mo Kα) = 1.643 mm-1, *Dcalc* = 1.858 g/mm3, 21935 reflections measured (6.02 ≤ 2Θ ≤ 60.3), 7625 unique (*R*int = 0.0379) which were used in all calculations. The final *R*1 was 0.0420 (>2sigma(I)) and *wR*2 was 0.0767 (all data).

This report has been created with Olex2, compiled on 2013.09.17 svn.r2790 for OlexSys. Please let us know if there are any errors or if you would like to have additional featrues.