

Table 1. Crystal data and structure refinement for 2.

|                                   |                                                        |                 |
|-----------------------------------|--------------------------------------------------------|-----------------|
| Identification code               | 2                                                      |                 |
| Empirical formula                 | C <sub>22</sub> H <sub>24</sub> Cl N O <sub>2</sub> Ru |                 |
| Formula weight                    | 470.94                                                 |                 |
| Temperature                       | 150(2) K                                               |                 |
| Wavelength                        | 0.71073 Å                                              |                 |
| Crystal system                    | Monoclinic                                             |                 |
| Space group                       | P 2 <sub>1</sub> /n                                    |                 |
| Unit cell dimensions              | a = 10.4657(4) Å                                       | α = 90°.        |
|                                   | b = 9.1505(3) Å                                        | β = 99.097(2)°. |
|                                   | c = 21.1478(8) Å                                       | γ = 90°.        |
| Volume                            | 1999.78(13) Å <sup>3</sup>                             |                 |
| Z                                 | 4                                                      |                 |
| Density (calculated)              | 1.564 Mg/m <sup>3</sup>                                |                 |
| Absorption coefficient            | 0.934 mm <sup>-1</sup>                                 |                 |
| F(000)                            | 960                                                    |                 |
| Crystal size                      | 0.18 x 0.14 x 0.12 mm <sup>3</sup>                     |                 |
| Theta range for data collection   | 1.95 to 28.75°.                                        |                 |
| Index ranges                      | -14 ≤ h ≤ 14, -12 ≤ k ≤ 12, -28 ≤ l ≤ 25               |                 |
| Reflections collected             | 28629                                                  |                 |
| Independent reflections           | 5176 [R(int) = 0.0263]                                 |                 |
| Completeness to theta = 28.75°    | 99.8 %                                                 |                 |
| Absorption correction             | Semi-empirical from equivalents                        |                 |
| Max. and min. transmission        | 0.8962 and 0.8499                                      |                 |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>            |                 |
| Data / restraints / parameters    | 5176 / 0 / 248                                         |                 |
| Goodness-of-fit on F <sup>2</sup> | 1.027                                                  |                 |
| Final R indices [I > 2σ(I)]       | R1 = 0.0208, wR2 = 0.0494                              |                 |
| R indices (all data)              | R1 = 0.0260, wR2 = 0.0520                              |                 |
| Largest diff. peak and hole       | 0.406 and -0.367 e.Å <sup>-3</sup>                     |                 |

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

|       | x       | y       | z       | U(eq) |
|-------|---------|---------|---------|-------|
| Ru(1) | 5663(1) | 3196(1) | 995(1)  | 20(1) |
| Cl(1) | 7674(1) | 4514(1) | 1072(1) | 29(1) |
| C(7)  | 5712(2) | 842(2)  | 869(1)  | 27(1) |
| C(8)  | 2495(2) | 3037(2) | 649(1)  | 27(1) |
| C(5)  | 3781(2) | 2389(2) | 547(1)  | 24(1) |
| C(6)  | 4437(2) | 1288(2) | 942(1)  | 26(1) |
| C(4)  | 4423(2) | 3004(2) | 60(1)   | 26(1) |
| C(3)  | 5674(2) | 2572(2) | -10(1)  | 27(1) |
| C(1)  | 7726(2) | 1126(2) | 349(1)  | 37(1) |
| C(9)  | 1416(2) | 2649(2) | 99(1)   | 37(1) |
| C(10) | 2112(2) | 2640(3) | 1286(1) | 43(1) |
| C(2)  | 6351(2) | 1486(2) | 402(1)  | 28(1) |
| N(1)  | 5962(1) | 3290(1) | 1981(1) | 21(1) |
| O(1)  | 4848(1) | 5222(1) | 1180(1) | 22(1) |
| C(16) | 4405(2) | 6982(2) | 1947(1) | 21(1) |
| C(15) | 4955(1) | 5577(2) | 1768(1) | 20(1) |
| C(14) | 5566(1) | 4590(2) | 2228(1) | 21(1) |
| C(12) | 6457(2) | 3218(2) | 3057(1) | 27(1) |
| C(13) | 5865(2) | 4552(2) | 2902(1) | 25(1) |
| C(11) | 6488(1) | 2472(2) | 2478(1) | 24(1) |
| C(17) | 3115(2) | 7365(2) | 1706(1) | 22(1) |
| C(21) | 5139(2) | 7919(2) | 2379(1) | 24(1) |
| C(18) | 2596(2) | 8650(2) | 1907(1) | 26(1) |
| C(20) | 4631(2) | 9220(2) | 2567(1) | 28(1) |
| C(19) | 3360(2) | 9570(2) | 2332(1) | 28(1) |
| O(2)  | 2434(1) | 6391(1) | 1297(1) | 29(1) |
| C(22) | 1089(2) | 6673(2) | 1098(1) | 35(1) |

Table 3. Bond lengths [Å] and angles [°] for 2.

|             |            |
|-------------|------------|
| Ru(1)-N(1)  | 2.0601(13) |
| Ru(1)-O(1)  | 2.1030(11) |
| Ru(1)-C(6)  | 2.1585(16) |
| Ru(1)-C(7)  | 2.1724(16) |
| Ru(1)-C(5)  | 2.1753(15) |
| Ru(1)-C(4)  | 2.1943(15) |
| Ru(1)-C(2)  | 2.1960(16) |
| Ru(1)-C(3)  | 2.2028(15) |
| Ru(1)-Cl(1) | 2.4092(4)  |
| C(7)-C(2)   | 1.406(2)   |
| C(7)-C(6)   | 1.427(2)   |
| C(8)-C(10)  | 1.510(3)   |
| C(8)-C(5)   | 1.517(2)   |
| C(8)-C(9)   | 1.529(2)   |
| C(5)-C(6)   | 1.415(2)   |
| C(5)-C(4)   | 1.432(2)   |
| C(4)-C(3)   | 1.397(2)   |
| C(3)-C(2)   | 1.434(2)   |
| C(1)-C(2)   | 1.498(2)   |
| N(1)-C(11)  | 1.3358(19) |
| N(1)-C(14)  | 1.3892(19) |
| O(1)-C(15)  | 1.2728(18) |
| C(16)-C(21) | 1.392(2)   |
| C(16)-C(17) | 1.410(2)   |
| C(16)-C(15) | 1.482(2)   |
| C(15)-C(14) | 1.406(2)   |
| C(14)-C(13) | 1.411(2)   |
| C(12)-C(13) | 1.384(2)   |
| C(12)-C(11) | 1.408(2)   |
| C(17)-O(2)  | 1.3621(19) |
| C(17)-C(18) | 1.390(2)   |
| C(21)-C(20) | 1.387(2)   |
| C(18)-C(19) | 1.388(2)   |
| C(20)-C(19) | 1.382(2)   |

|                  |            |
|------------------|------------|
| O(2)-C(22)       | 1.4277(19) |
| N(1)-Ru(1)-O(1)  | 77.09(4)   |
| N(1)-Ru(1)-C(6)  | 94.59(6)   |
| O(1)-Ru(1)-C(6)  | 117.86(5)  |
| N(1)-Ru(1)-C(7)  | 99.37(6)   |
| O(1)-Ru(1)-C(7)  | 156.24(5)  |
| C(6)-Ru(1)-C(7)  | 38.48(6)   |
| N(1)-Ru(1)-C(5)  | 115.91(6)  |
| O(1)-Ru(1)-C(5)  | 90.81(5)   |
| C(6)-Ru(1)-C(5)  | 38.11(6)   |
| C(7)-Ru(1)-C(5)  | 69.35(6)   |
| N(1)-Ru(1)-C(4)  | 152.74(6)  |
| O(1)-Ru(1)-C(4)  | 92.21(5)   |
| C(6)-Ru(1)-C(4)  | 68.08(6)   |
| C(7)-Ru(1)-C(4)  | 80.33(6)   |
| C(5)-Ru(1)-C(4)  | 38.25(6)   |
| N(1)-Ru(1)-C(2)  | 126.60(6)  |
| O(1)-Ru(1)-C(2)  | 155.95(5)  |
| C(6)-Ru(1)-C(2)  | 68.91(6)   |
| C(7)-Ru(1)-C(2)  | 37.54(6)   |
| C(5)-Ru(1)-C(2)  | 82.28(6)   |
| C(4)-Ru(1)-C(2)  | 68.22(6)   |
| N(1)-Ru(1)-C(3)  | 164.61(6)  |
| O(1)-Ru(1)-C(3)  | 118.13(5)  |
| C(6)-Ru(1)-C(3)  | 80.45(6)   |
| C(7)-Ru(1)-C(3)  | 67.71(6)   |
| C(5)-Ru(1)-C(3)  | 68.54(6)   |
| C(4)-Ru(1)-C(3)  | 37.04(6)   |
| C(2)-Ru(1)-C(3)  | 38.05(6)   |
| N(1)-Ru(1)-Cl(1) | 85.41(4)   |
| O(1)-Ru(1)-Cl(1) | 85.52(3)   |
| C(6)-Ru(1)-Cl(1) | 156.07(5)  |
| C(7)-Ru(1)-Cl(1) | 117.86(5)  |
| C(5)-Ru(1)-Cl(1) | 157.00(4)  |
| C(4)-Ru(1)-Cl(1) | 119.11(5)  |

|                   |            |
|-------------------|------------|
| C(2)-Ru(1)-Cl(1)  | 91.90(5)   |
| C(3)-Ru(1)-Cl(1)  | 93.26(5)   |
| C(2)-C(7)-C(6)    | 120.82(15) |
| C(2)-C(7)-Ru(1)   | 72.14(9)   |
| C(6)-C(7)-Ru(1)   | 70.23(9)   |
| C(10)-C(8)-C(5)   | 113.54(14) |
| C(10)-C(8)-C(9)   | 110.71(16) |
| C(5)-C(8)-C(9)    | 111.53(14) |
| C(6)-C(5)-C(4)    | 117.74(15) |
| C(6)-C(5)-C(8)    | 123.60(15) |
| C(4)-C(5)-C(8)    | 118.44(14) |
| C(6)-C(5)-Ru(1)   | 70.30(9)   |
| C(4)-C(5)-Ru(1)   | 71.59(9)   |
| C(8)-C(5)-Ru(1)   | 124.62(11) |
| C(5)-C(6)-C(7)    | 120.97(15) |
| C(5)-C(6)-Ru(1)   | 71.58(9)   |
| C(7)-C(6)-Ru(1)   | 71.29(9)   |
| C(3)-C(4)-C(5)    | 121.29(15) |
| C(3)-C(4)-Ru(1)   | 71.81(9)   |
| C(5)-C(4)-Ru(1)   | 70.16(9)   |
| C(4)-C(3)-C(2)    | 120.85(15) |
| C(4)-C(3)-Ru(1)   | 71.15(9)   |
| C(2)-C(3)-Ru(1)   | 70.72(9)   |
| C(7)-C(2)-C(3)    | 118.27(15) |
| C(7)-C(2)-C(1)    | 121.97(16) |
| C(3)-C(2)-C(1)    | 119.68(16) |
| C(7)-C(2)-Ru(1)   | 70.32(9)   |
| C(3)-C(2)-Ru(1)   | 71.23(9)   |
| C(1)-C(2)-Ru(1)   | 127.24(12) |
| C(11)-N(1)-C(14)  | 107.08(13) |
| C(11)-N(1)-Ru(1)  | 138.62(11) |
| C(14)-N(1)-Ru(1)  | 114.24(10) |
| C(15)-O(1)-Ru(1)  | 115.49(9)  |
| C(21)-C(16)-C(17) | 118.79(14) |
| C(21)-C(16)-C(15) | 120.40(14) |
| C(17)-C(16)-C(15) | 120.76(13) |

|                   |            |
|-------------------|------------|
| O(1)-C(15)-C(14)  | 118.27(14) |
| O(1)-C(15)-C(16)  | 119.58(13) |
| C(14)-C(15)-C(16) | 122.13(13) |
| N(1)-C(14)-C(15)  | 114.76(13) |
| N(1)-C(14)-C(13)  | 109.13(13) |
| C(15)-C(14)-C(13) | 136.08(15) |
| C(13)-C(12)-C(11) | 107.05(14) |
| C(12)-C(13)-C(14) | 106.28(14) |
| N(1)-C(11)-C(12)  | 110.45(14) |
| O(2)-C(17)-C(18)  | 123.87(14) |
| O(2)-C(17)-C(16)  | 116.23(14) |
| C(18)-C(17)-C(16) | 119.85(14) |
| C(20)-C(21)-C(16) | 121.29(15) |
| C(19)-C(18)-C(17) | 119.89(15) |
| C(19)-C(20)-C(21) | 119.16(15) |
| C(20)-C(19)-C(18) | 120.98(15) |
| C(17)-O(2)-C(22)  | 117.49(13) |

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Symmetry transformations used to generate equivalent atoms:

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

|       | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|-------|----------|----------|----------|----------|----------|----------|
| Ru(1) | 21(1)    | 20(1)    | 17(1)    | 0(1)     | -1(1)    | 3(1)     |
| Cl(1) | 24(1)    | 32(1)    | 31(1)    | 1(1)     | 2(1)     | -2(1)    |
| C(7)  | 32(1)    | 21(1)    | 25(1)    | -1(1)    | -2(1)    | 4(1)     |
| C(8)  | 24(1)    | 27(1)    | 28(1)    | -4(1)    | -3(1)    | 2(1)     |
| C(5)  | 25(1)    | 23(1)    | 22(1)    | -5(1)    | -3(1)    | 0(1)     |
| C(6)  | 29(1)    | 23(1)    | 24(1)    | -2(1)    | 0(1)     | -2(1)    |
| C(4)  | 30(1)    | 25(1)    | 19(1)    | -2(1)    | -4(1)    | 1(1)     |
| C(3)  | 34(1)    | 26(1)    | 20(1)    | -3(1)    | 2(1)     | 2(1)     |
| C(1)  | 36(1)    | 39(1)    | 38(1)    | -5(1)    | 7(1)     | 11(1)    |
| C(9)  | 26(1)    | 45(1)    | 37(1)    | -8(1)    | -5(1)    | 1(1)     |
| C(10) | 38(1)    | 58(1)    | 34(1)    | 1(1)     | 9(1)     | 14(1)    |
| C(2)  | 32(1)    | 26(1)    | 24(1)    | -5(1)    | 1(1)     | 6(1)     |
| N(1)  | 19(1)    | 23(1)    | 20(1)    | 1(1)     | 0(1)     | 1(1)     |
| O(1)  | 24(1)    | 24(1)    | 19(1)    | -1(1)    | -1(1)    | 4(1)     |
| C(16) | 20(1)    | 24(1)    | 20(1)    | 1(1)     | 4(1)     | 1(1)     |
| C(15) | 15(1)    | 24(1)    | 21(1)    | -2(1)    | 1(1)     | -1(1)    |
| C(14) | 19(1)    | 24(1)    | 20(1)    | 0(1)     | 1(1)     | -1(1)    |
| C(12) | 24(1)    | 36(1)    | 20(1)    | 6(1)     | 0(1)     | -2(1)    |
| C(13) | 22(1)    | 33(1)    | 20(1)    | 0(1)     | 2(1)     | -3(1)    |
| C(11) | 18(1)    | 26(1)    | 26(1)    | 6(1)     | 0(1)     | -1(1)    |
| C(17) | 21(1)    | 24(1)    | 20(1)    | 2(1)     | 3(1)     | 1(1)     |
| C(21) | 20(1)    | 28(1)    | 24(1)    | -1(1)    | 3(1)     | -2(1)    |
| C(18) | 25(1)    | 28(1)    | 26(1)    | 3(1)     | 5(1)     | 7(1)     |
| C(20) | 32(1)    | 27(1)    | 25(1)    | -4(1)    | 6(1)     | -4(1)    |
| C(19) | 35(1)    | 26(1)    | 25(1)    | -1(1)    | 8(1)     | 6(1)     |
| O(2)  | 19(1)    | 31(1)    | 33(1)    | -5(1)    | -6(1)    | 4(1)     |
| C(22) | 21(1)    | 36(1)    | 44(1)    | 2(1)     | -8(1)    | 2(1)     |

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for 2.

|        | x    | y     | z    | U(eq) |
|--------|------|-------|------|-------|
| H(7)   | 6135 | 99    | 1139 | 32    |
| H(8)   | 2596 | 4124  | 645  | 33    |
| H(6)   | 4023 | 840   | 1261 | 31    |
| H(4)   | 3991 | 3719  | -222 | 31    |
| H(3)   | 6080 | 3004  | -335 | 32    |
| H(1A)  | 8070 | 433   | 687  | 56    |
| H(1B)  | 8247 | 2022  | 396  | 56    |
| H(1C)  | 7763 | 688   | -71  | 56    |
| H(9A)  | 1247 | 1596  | 104  | 56    |
| H(9B)  | 1682 | 2918  | -309 | 56    |
| H(9C)  | 628  | 3184  | 151  | 56    |
| H(10A) | 1935 | 1589  | 1296 | 64    |
| H(10B) | 1333 | 3185  | 1344 | 64    |
| H(10C) | 2818 | 2888  | 1631 | 64    |
| H(12)  | 6782 | 2873  | 3475 | 32    |
| H(13)  | 5694 | 5293  | 3192 | 30    |
| H(11)  | 6834 | 1520  | 2445 | 28    |
| H(21)  | 6006 | 7663  | 2549 | 29    |
| H(18)  | 1720 | 8898  | 1754 | 31    |
| H(20)  | 5150 | 9862  | 2853 | 33    |
| H(19)  | 3003 | 10453 | 2463 | 34    |
| H(22A) | 660  | 6770  | 1476 | 52    |
| H(22B) | 700  | 5862  | 832  | 52    |
| H(22C) | 984  | 7581  | 849  | 52    |





Table 1. Crystal data and structure refinement for 3.

|                                   |                                                                       |                 |
|-----------------------------------|-----------------------------------------------------------------------|-----------------|
| Identification code               | 3                                                                     |                 |
| Empirical formula                 | C <sub>53</sub> H <sub>48</sub> Cl N O <sub>4</sub> P <sub>2</sub> Ru |                 |
| Formula weight                    | 961.38                                                                |                 |
| Temperature                       | 150(2) K                                                              |                 |
| Wavelength                        | 0.71073 Å                                                             |                 |
| Crystal system                    | Monoclinic                                                            |                 |
| Space group                       | P2 <sub>1</sub> /n                                                    |                 |
| Unit cell dimensions              | a = 10.2279(5) Å                                                      | α = 90°.        |
|                                   | b = 17.5822(9) Å                                                      | β = 97.693(3)°. |
|                                   | c = 25.9234(13) Å                                                     | γ = 90°.        |
| Volume                            | 4619.8(4) Å <sup>3</sup>                                              |                 |
| Z                                 | 4                                                                     |                 |
| Density (calculated)              | 1.382 Mg/m <sup>3</sup>                                               |                 |
| Absorption coefficient            | 0.513 mm <sup>-1</sup>                                                |                 |
| F(000)                            | 1824                                                                  |                 |
| Crystal size                      | 0.18 x 0.14 x 0.12 mm <sup>3</sup>                                    |                 |
| Theta range for data collection   | 1.40 to 25.00°.                                                       |                 |
| Index ranges                      | -12 ≤ h ≤ 12, -20 ≤ k ≤ 20, -30 ≤ l ≤ 30                              |                 |
| Reflections collected             | 49633                                                                 |                 |
| Independent reflections           | 8132 [R(int) = 0.0979]                                                |                 |
| Completeness to theta = 25.00°    | 100.0 %                                                               |                 |
| Absorption correction             | Semi-empirical from equivalents                                       |                 |
| Max. and min. transmission        | 0.9410 and 0.9133                                                     |                 |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                           |                 |
| Data / restraints / parameters    | 8132 / 0 / 560                                                        |                 |
| Goodness-of-fit on F <sup>2</sup> | 0.880                                                                 |                 |
| Final R indices [I > 2σ(I)]       | R1 = 0.0591, wR2 = 0.1682                                             |                 |
| R indices (all data)              | R1 = 0.0879, wR2 = 0.1925                                             |                 |
| Largest diff. peak and hole       | 0.811 and -0.925 e.Å <sup>-3</sup>                                    |                 |

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

|       | x        | y        | z        | U(eq) |
|-------|----------|----------|----------|-------|
| Ru(1) | 9642(1)  | 8351(1)  | 8102(1)  | 21(1) |
| Cl(1) | 10933(1) | 7559(1)  | 7598(1)  | 31(1) |
| P(1)  | 8581(1)  | 8980(1)  | 7333(1)  | 22(1) |
| P(2)  | 10657(1) | 7770(1)  | 8889(1)  | 22(1) |
| N(1)  | 8886(4)  | 9200(3)  | 8508(2)  | 23(1) |
| O(1)  | 11228(4) | 9153(2)  | 8189(1)  | 23(1) |
| O(2)  | 10725(5) | 11242(3) | 8022(2)  | 39(1) |
| C(50) | 8197(6)  | 7721(4)  | 8093(2)  | 30(1) |
| O(4)  | 7293(5)  | 7361(3)  | 8114(2)  | 45(1) |
| C(1)  | 7073(5)  | 9442(3)  | 7472(2)  | 23(1) |
| C(2)  | 7040(6)  | 10200(3) | 7645(2)  | 28(1) |
| C(3)  | 5876(6)  | 10510(4) | 7770(2)  | 34(2) |
| C(4)  | 4752(6)  | 10076(4) | 7740(2)  | 38(2) |
| C(5)  | 4771(6)  | 9324(4)  | 7596(2)  | 34(2) |
| O(3)  | 3010(9)  | 3975(5)  | 9738(4)  | 98(2) |
| C(6)  | 5928(5)  | 9010(4)  | 7455(2)  | 28(1) |
| C(7)  | 9546(6)  | 9704(4)  | 7052(2)  | 28(1) |
| C(8)  | 10891(6) | 9571(4)  | 7063(2)  | 32(1) |
| C(9)  | 11686(7) | 10092(4) | 6848(3)  | 42(2) |
| C(10) | 11142(7) | 10744(4) | 6614(3)  | 46(2) |
| C(11) | 9814(7)  | 10873(4) | 6591(3)  | 44(2) |
| C(12) | 9008(6)  | 10364(4) | 6805(3)  | 35(2) |
| C(13) | 7917(6)  | 8398(3)  | 6773(2)  | 26(1) |
| C(14) | 7209(7)  | 8741(4)  | 6338(3)  | 40(2) |
| C(15) | 6614(7)  | 8308(5)  | 5928(3)  | 46(2) |
| C(16) | 6733(7)  | 7531(4)  | 5944(3)  | 38(2) |
| C(17) | 7428(7)  | 7184(4)  | 6363(3)  | 40(2) |
| C(18) | 8036(6)  | 7621(4)  | 6779(3)  | 34(2) |
| C(19) | 9830(6)  | 8008(4)  | 9449(2)  | 27(1) |
| C(20) | 9869(7)  | 8757(4)  | 9634(2)  | 38(2) |
| C(21) | 9170(8)  | 8969(4)  | 10032(3) | 44(2) |

|       |          |          |           |         |
|-------|----------|----------|-----------|---------|
| C(22) | 8393(7)  | 8443(5)  | 10247(3)  | 47(2)   |
| C(23) | 8342(7)  | 7712(5)  | 10065(3)  | 49(2)   |
| C(24) | 9041(6)  | 7497(4)  | 9668(3)   | 36(2)   |
| C(25) | 12399(6) | 8020(3)  | 9081(2)   | 28(1)   |
| C(26) | 13243(6) | 7960(4)  | 8709(3)   | 32(1)   |
| C(27) | 14568(6) | 8100(4)  | 8833(3)   | 39(2)   |
| C(28) | 15076(7) | 8306(4)  | 9333(3)   | 47(2)   |
| C(29) | 14256(7) | 8377(5)  | 9709(3)   | 52(2)   |
| C(30) | 12911(7) | 8231(4)  | 9586(2)   | 39(2)   |
| C(31) | 10725(5) | 6736(3)  | 8937(2)   | 25(1)   |
| C(32) | 11360(7) | 6403(4)  | 9390(3)   | 36(2)   |
| C(33) | 11363(7) | 5629(4)  | 9456(3)   | 42(2)   |
| C(34) | 10704(7) | 5163(4)  | 9067(3)   | 39(2)   |
| C(35) | 10088(6) | 5476(4)  | 8619(2)   | 33(1)   |
| C(36) | 10102(6) | 6268(3)  | 8549(2)   | 27(1)   |
| C(37) | 7806(6)  | 9357(4)  | 8729(2)   | 28(1)   |
| C(38) | 7910(6)  | 10087(4) | 8951(2)   | 32(1)   |
| C(39) | 9087(6)  | 10388(3) | 8859(2)   | 28(1)   |
| C(40) | 9704(5)  | 9838(3)  | 8583(2)   | 23(1)   |
| C(41) | 10944(5) | 9766(3)  | 8416(2)   | 24(1)   |
| C(42) | 12001(5) | 10349(3) | 8532(2)   | 23(1)   |
| C(43) | 11874(6) | 11088(4) | 8334(2)   | 30(1)   |
| C(44) | 10566(8) | 11992(4) | 7807(3)   | 54(2)   |
| C(45) | 12907(7) | 11600(4) | 8452(3)   | 37(2)   |
| C(46) | 14034(7) | 11383(4) | 8774(3)   | 39(2)   |
| C(47) | 14165(6) | 10660(4) | 8972(3)   | 37(2)   |
| C(48) | 13147(6) | 10139(4) | 8848(2)   | 29(1)   |
| C(54) | 3834(16) | 3942(8)  | 10199(6)  | 128(6)  |
| C(53) | 5115(16) | 3795(10) | 10099(10) | 164(9)  |
| C(51) | 3683(19) | 3869(11) | 9317(6)   | 146(7)  |
| C(52) | 4960(20) | 3557(15) | 9523(10)  | 211(12) |

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

|             |            |
|-------------|------------|
| Ru(1)-C(50) | 1.845(7)   |
| Ru(1)-N(1)  | 2.038(5)   |
| Ru(1)-O(1)  | 2.139(4)   |
| Ru(1)-P(2)  | 2.3908(15) |
| Ru(1)-P(1)  | 2.4058(15) |
| Ru(1)-Cl(1) | 2.4185(15) |
| P(1)-C(1)   | 1.821(6)   |
| P(1)-C(13)  | 1.832(6)   |
| P(1)-C(7)   | 1.823(6)   |
| P(2)-C(31)  | 1.824(6)   |
| P(2)-C(19)  | 1.825(6)   |
| P(2)-C(25)  | 1.838(6)   |
| N(1)-C(37)  | 1.338(7)   |
| N(1)-C(40)  | 1.398(7)   |
| O(1)-C(41)  | 1.280(7)   |
| O(2)-C(43)  | 1.362(7)   |
| O(2)-C(44)  | 1.432(8)   |
| C(50)-O(4)  | 1.128(8)   |
| C(1)-C(6)   | 1.392(8)   |
| C(1)-C(2)   | 1.408(8)   |
| C(2)-C(3)   | 1.387(8)   |
| C(2)-H(2)   | 0.9300     |
| C(3)-C(4)   | 1.374(10)  |
| C(3)-H(3)   | 0.9300     |
| C(4)-C(5)   | 1.375(10)  |
| C(4)-H(4)   | 0.9300     |
| C(5)-C(6)   | 1.398(9)   |
| C(5)-H(5)   | 0.9300     |
| O(3)-C(54)  | 1.370(14)  |
| O(3)-C(51)  | 1.377(18)  |
| C(6)-H(6)   | 0.9300     |
| C(7)-C(8)   | 1.391(8)   |
| C(7)-C(12)  | 1.401(9)   |
| C(8)-C(9)   | 1.390(9)   |

|             |           |
|-------------|-----------|
| C(8)-H(8)   | 0.9300    |
| C(9)-C(10)  | 1.378(10) |
| C(9)-H(9)   | 0.9300    |
| C(10)-C(11) | 1.370(10) |
| C(10)-H(10) | 0.9300    |
| C(11)-C(12) | 1.382(9)  |
| C(11)-H(11) | 0.9300    |
| C(12)-H(12) | 0.9300    |
| C(13)-C(18) | 1.372(9)  |
| C(13)-C(14) | 1.393(9)  |
| C(14)-C(15) | 1.380(10) |
| C(14)-H(14) | 0.9300    |
| C(15)-C(16) | 1.372(10) |
| C(15)-H(15) | 0.9300    |
| C(16)-C(17) | 1.361(10) |
| C(16)-H(16) | 0.9300    |
| C(17)-C(18) | 1.400(9)  |
| C(17)-H(17) | 0.9300    |
| C(18)-H(18) | 0.9300    |
| C(19)-C(24) | 1.379(9)  |
| C(19)-C(20) | 1.399(9)  |
| C(20)-C(21) | 1.383(10) |
| C(20)-H(20) | 0.9300    |
| C(21)-C(22) | 1.386(11) |
| C(21)-H(21) | 0.9300    |
| C(22)-C(23) | 1.368(11) |
| C(22)-H(22) | 0.9300    |
| C(23)-C(24) | 1.382(10) |
| C(23)-H(23) | 0.9300    |
| C(24)-H(24) | 0.9300    |
| C(25)-C(26) | 1.383(9)  |
| C(25)-C(30) | 1.393(9)  |
| C(26)-C(27) | 1.373(9)  |
| C(26)-H(26) | 0.9300    |
| C(27)-C(28) | 1.378(10) |
| C(27)-H(27) | 0.9300    |

|              |           |
|--------------|-----------|
| C(28)-C(29)  | 1.375(11) |
| C(28)-H(28)  | 0.9300    |
| C(29)-C(30)  | 1.394(10) |
| C(29)-H(29)  | 0.9300    |
| C(30)-H(30)  | 0.9300    |
| C(31)-C(36)  | 1.385(8)  |
| C(31)-C(32)  | 1.393(8)  |
| C(32)-C(33)  | 1.371(10) |
| C(32)-H(32)  | 0.9300    |
| C(33)-C(34)  | 1.402(9)  |
| C(33)-H(33)  | 0.9300    |
| C(34)-C(35)  | 1.360(9)  |
| C(34)-H(34)  | 0.9300    |
| C(35)-C(36)  | 1.406(9)  |
| C(35)-H(35)  | 0.9300    |
| C(36)-H(36)  | 0.9300    |
| C(37)-C(38)  | 1.405(9)  |
| C(37)-H(37)  | 0.9300    |
| C(38)-C(39)  | 1.365(9)  |
| C(38)-H(38)  | 0.9300    |
| C(39)-C(40)  | 1.403(8)  |
| C(39)-H(39)  | 0.9300    |
| C(40)-C(41)  | 1.400(8)  |
| C(41)-C(42)  | 1.490(8)  |
| C(42)-C(48)  | 1.387(8)  |
| C(42)-C(43)  | 1.396(9)  |
| C(43)-C(45)  | 1.391(9)  |
| C(44)-H(44A) | 0.9600    |
| C(44)-H(44B) | 0.9600    |
| C(44)-H(44C) | 0.9600    |
| C(45)-C(46)  | 1.383(10) |
| C(45)-H(45)  | 0.9300    |
| C(46)-C(47)  | 1.371(10) |
| C(46)-H(46)  | 0.9300    |
| C(47)-C(48)  | 1.392(9)  |
| C(47)-H(47)  | 0.9300    |

|                   |            |
|-------------------|------------|
| C(48)-H(48)       | 0.9300     |
| C(54)-C(53)       | 1.39(2)    |
| C(54)-H(54A)      | 0.9700     |
| C(54)-H(54B)      | 0.9700     |
| C(53)-C(52)       | 1.54(3)    |
| C(53)-H(53A)      | 0.9700     |
| C(53)-H(53B)      | 0.9700     |
| C(51)-C(52)       | 1.45(2)    |
| C(51)-H(51A)      | 0.9700     |
| C(51)-H(51B)      | 0.9700     |
| C(52)-H(52A)      | 0.9700     |
| C(52)-H(52B)      | 0.9700     |
|                   |            |
| C(50)-Ru(1)-N(1)  | 95.0(2)    |
| C(50)-Ru(1)-O(1)  | 172.9(2)   |
| N(1)-Ru(1)-O(1)   | 78.32(16)  |
| C(50)-Ru(1)-P(2)  | 90.52(18)  |
| N(1)-Ru(1)-P(2)   | 91.33(13)  |
| O(1)-Ru(1)-P(2)   | 87.45(11)  |
| C(50)-Ru(1)-P(1)  | 89.66(18)  |
| N(1)-Ru(1)-P(1)   | 86.05(13)  |
| O(1)-Ru(1)-P(1)   | 92.06(11)  |
| P(2)-Ru(1)-P(1)   | 177.38(5)  |
| C(50)-Ru(1)-Cl(1) | 98.2(2)    |
| N(1)-Ru(1)-Cl(1)  | 166.70(14) |
| O(1)-Ru(1)-Cl(1)  | 88.61(11)  |
| P(2)-Ru(1)-Cl(1)  | 90.48(5)   |
| P(1)-Ru(1)-Cl(1)  | 92.08(5)   |
| C(1)-P(1)-C(13)   | 99.9(3)    |
| C(1)-P(1)-C(7)    | 106.6(3)   |
| C(13)-P(1)-C(7)   | 103.6(3)   |
| C(1)-P(1)-Ru(1)   | 109.97(19) |
| C(13)-P(1)-Ru(1)  | 118.6(2)   |
| C(7)-P(1)-Ru(1)   | 116.36(19) |
| C(31)-P(2)-C(19)  | 101.1(3)   |
| C(31)-P(2)-C(25)  | 101.1(3)   |



|                  |            |
|------------------|------------|
| C(19)-P(2)-C(25) | 105.4(3)   |
| C(31)-P(2)-Ru(1) | 119.5(2)   |
| C(19)-P(2)-Ru(1) | 112.77(19) |
| C(25)-P(2)-Ru(1) | 115.1(2)   |
| C(37)-N(1)-C(40) | 106.7(5)   |
| C(37)-N(1)-Ru(1) | 139.8(4)   |
| C(40)-N(1)-Ru(1) | 113.5(4)   |
| C(41)-O(1)-Ru(1) | 112.9(3)   |
| C(43)-O(2)-C(44) | 117.3(5)   |
| O(4)-C(50)-Ru(1) | 175.7(6)   |
| C(6)-C(1)-C(2)   | 118.1(5)   |
| C(6)-C(1)-P(1)   | 118.8(5)   |
| C(2)-C(1)-P(1)   | 122.8(4)   |
| C(3)-C(2)-C(1)   | 120.3(6)   |
| C(3)-C(2)-H(2)   | 119.9      |
| C(1)-C(2)-H(2)   | 119.9      |
| C(4)-C(3)-C(2)   | 120.5(6)   |
| C(4)-C(3)-H(3)   | 119.8      |
| C(2)-C(3)-H(3)   | 119.8      |
| C(3)-C(4)-C(5)   | 120.5(6)   |
| C(3)-C(4)-H(4)   | 119.8      |
| C(5)-C(4)-H(4)   | 119.8      |
| C(4)-C(5)-C(6)   | 119.6(6)   |
| C(4)-C(5)-H(5)   | 120.2      |
| C(6)-C(5)-H(5)   | 120.2      |
| C(54)-O(3)-C(51) | 111.8(13)  |
| C(1)-C(6)-C(5)   | 121.0(6)   |
| C(1)-C(6)-H(6)   | 119.5      |
| C(5)-C(6)-H(6)   | 119.5      |
| C(8)-C(7)-C(12)  | 118.3(6)   |
| C(8)-C(7)-P(1)   | 117.5(5)   |
| C(12)-C(7)-P(1)  | 124.1(5)   |
| C(7)-C(8)-C(9)   | 120.7(6)   |
| C(7)-C(8)-H(8)   | 119.6      |
| C(9)-C(8)-H(8)   | 119.6      |
| C(10)-C(9)-C(8)  | 120.1(7)   |

|                   |          |
|-------------------|----------|
| C(10)-C(9)-H(9)   | 120.0    |
| C(8)-C(9)-H(9)    | 120.0    |
| C(11)-C(10)-C(9)  | 119.8(7) |
| C(11)-C(10)-H(10) | 120.1    |
| C(9)-C(10)-H(10)  | 120.1    |
| C(10)-C(11)-C(12) | 121.1(7) |
| C(10)-C(11)-H(11) | 119.5    |
| C(12)-C(11)-H(11) | 119.5    |
| C(11)-C(12)-C(7)  | 120.0(6) |
| C(11)-C(12)-H(12) | 120.0    |
| C(7)-C(12)-H(12)  | 120.0    |
| C(18)-C(13)-C(14) | 118.5(6) |
| C(18)-C(13)-P(1)  | 121.6(5) |
| C(14)-C(13)-P(1)  | 119.9(5) |
| C(15)-C(14)-C(13) | 120.8(7) |
| C(15)-C(14)-H(14) | 119.6    |
| C(13)-C(14)-H(14) | 119.6    |
| C(16)-C(15)-C(14) | 119.9(7) |
| C(16)-C(15)-H(15) | 120.0    |
| C(14)-C(15)-H(15) | 120.0    |
| C(17)-C(16)-C(15) | 120.3(6) |
| C(17)-C(16)-H(16) | 119.8    |
| C(15)-C(16)-H(16) | 119.8    |
| C(16)-C(17)-C(18) | 120.0(6) |
| C(16)-C(17)-H(17) | 120.0    |
| C(18)-C(17)-H(17) | 120.0    |
| C(13)-C(18)-C(17) | 120.5(6) |
| C(13)-C(18)-H(18) | 119.8    |
| C(17)-C(18)-H(18) | 119.8    |
| C(24)-C(19)-C(20) | 117.6(6) |
| C(24)-C(19)-P(2)  | 122.5(5) |
| C(20)-C(19)-P(2)  | 119.5(5) |
| C(21)-C(20)-C(19) | 121.0(7) |
| C(21)-C(20)-H(20) | 119.5    |
| C(19)-C(20)-H(20) | 119.5    |
| C(22)-C(21)-C(20) | 120.1(7) |

|                   |          |
|-------------------|----------|
| C(22)-C(21)-H(21) | 119.9    |
| C(20)-C(21)-H(21) | 119.9    |
| C(23)-C(22)-C(21) | 119.0(7) |
| C(23)-C(22)-H(22) | 120.5    |
| C(21)-C(22)-H(22) | 120.5    |
| C(22)-C(23)-C(24) | 121.0(7) |
| C(22)-C(23)-H(23) | 119.5    |
| C(24)-C(23)-H(23) | 119.5    |
| C(19)-C(24)-C(23) | 121.2(7) |
| C(19)-C(24)-H(24) | 119.4    |
| C(23)-C(24)-H(24) | 119.4    |
| C(26)-C(25)-C(30) | 119.0(6) |
| C(26)-C(25)-P(2)  | 117.7(5) |
| C(30)-C(25)-P(2)  | 123.2(5) |
| C(27)-C(26)-C(25) | 120.8(6) |
| C(27)-C(26)-H(26) | 119.6    |
| C(25)-C(26)-H(26) | 119.6    |
| C(26)-C(27)-C(28) | 120.3(7) |
| C(26)-C(27)-H(27) | 119.9    |
| C(28)-C(27)-H(27) | 119.9    |
| C(29)-C(28)-C(27) | 120.1(6) |
| C(29)-C(28)-H(28) | 120.0    |
| C(27)-C(28)-H(28) | 120.0    |
| C(28)-C(29)-C(30) | 119.9(7) |
| C(28)-C(29)-H(29) | 120.0    |
| C(30)-C(29)-H(29) | 120.0    |
| C(29)-C(30)-C(25) | 120.0(7) |
| C(29)-C(30)-H(30) | 120.0    |
| C(25)-C(30)-H(30) | 120.0    |
| C(36)-C(31)-C(32) | 118.6(6) |
| C(36)-C(31)-P(2)  | 122.2(4) |
| C(32)-C(31)-P(2)  | 119.0(5) |
| C(33)-C(32)-C(31) | 121.0(6) |
| C(33)-C(32)-H(32) | 119.5    |
| C(31)-C(32)-H(32) | 119.5    |
| C(32)-C(33)-C(34) | 119.9(6) |

|                     |          |
|---------------------|----------|
| C(32)-C(33)-H(33)   | 120.1    |
| C(34)-C(33)-H(33)   | 120.1    |
| C(35)-C(34)-C(33)   | 120.0(6) |
| C(35)-C(34)-H(34)   | 120.0    |
| C(33)-C(34)-H(34)   | 120.0    |
| C(34)-C(35)-C(36)   | 119.9(6) |
| C(34)-C(35)-H(35)   | 120.0    |
| C(36)-C(35)-H(35)   | 120.0    |
| C(31)-C(36)-C(35)   | 120.5(6) |
| C(31)-C(36)-H(36)   | 119.8    |
| C(35)-C(36)-H(36)   | 119.8    |
| N(1)-C(37)-C(38)    | 110.1(5) |
| N(1)-C(37)-H(37)    | 125.0    |
| C(38)-C(37)-H(37)   | 125.0    |
| C(39)-C(38)-C(37)   | 107.6(5) |
| C(39)-C(38)-H(38)   | 126.2    |
| C(37)-C(38)-H(38)   | 126.2    |
| C(38)-C(39)-C(40)   | 106.8(5) |
| C(38)-C(39)-H(39)   | 126.6    |
| C(40)-C(39)-H(39)   | 126.6    |
| N(1)-C(40)-C(39)    | 108.8(5) |
| N(1)-C(40)-C(41)    | 115.8(5) |
| C(39)-C(40)-C(41)   | 135.1(6) |
| O(1)-C(41)-C(40)    | 119.3(5) |
| O(1)-C(41)-C(42)    | 117.9(5) |
| C(40)-C(41)-C(42)   | 122.6(5) |
| C(48)-C(42)-C(43)   | 119.6(5) |
| C(48)-C(42)-C(41)   | 118.0(5) |
| C(43)-C(42)-C(41)   | 122.4(5) |
| O(2)-C(43)-C(45)    | 124.8(6) |
| O(2)-C(43)-C(42)    | 115.7(5) |
| C(45)-C(43)-C(42)   | 119.5(6) |
| O(2)-C(44)-H(44A)   | 109.5    |
| O(2)-C(44)-H(44B)   | 109.5    |
| H(44A)-C(44)-H(44B) | 109.5    |
| O(2)-C(44)-H(44C)   | 109.5    |

|                     |           |
|---------------------|-----------|
| H(44A)-C(44)-H(44C) | 109.5     |
| H(44B)-C(44)-H(44C) | 109.5     |
| C(43)-C(45)-C(46)   | 120.0(6)  |
| C(43)-C(45)-H(45)   | 120.0     |
| C(46)-C(45)-H(45)   | 120.0     |
| C(47)-C(46)-C(45)   | 120.9(6)  |
| C(47)-C(46)-H(46)   | 119.5     |
| C(45)-C(46)-H(46)   | 119.5     |
| C(46)-C(47)-C(48)   | 119.4(6)  |
| C(46)-C(47)-H(47)   | 120.3     |
| C(48)-C(47)-H(47)   | 120.3     |
| C(47)-C(48)-C(42)   | 120.5(6)  |
| C(47)-C(48)-H(48)   | 119.7     |
| C(42)-C(48)-H(48)   | 119.7     |
| O(3)-C(54)-C(53)    | 109.2(16) |
| O(3)-C(54)-H(54A)   | 109.8     |
| C(53)-C(54)-H(54A)  | 109.8     |
| O(3)-C(54)-H(54B)   | 109.8     |
| C(53)-C(54)-H(54B)  | 109.8     |
| H(54A)-C(54)-H(54B) | 108.3     |
| C(54)-C(53)-C(52)   | 104.8(15) |
| C(54)-C(53)-H(53A)  | 110.8     |
| C(52)-C(53)-H(53A)  | 110.8     |
| C(54)-C(53)-H(53B)  | 110.8     |
| C(52)-C(53)-H(53B)  | 110.8     |
| H(53A)-C(53)-H(53B) | 108.9     |
| O(3)-C(51)-C(52)    | 106.3(14) |
| O(3)-C(51)-H(51A)   | 110.5     |
| C(52)-C(51)-H(51A)  | 110.5     |
| O(3)-C(51)-H(51B)   | 110.5     |
| C(52)-C(51)-H(51B)  | 110.5     |
| H(51A)-C(51)-H(51B) | 108.7     |
| C(51)-C(52)-C(53)   | 102.9(14) |
| C(51)-C(52)-H(52A)  | 111.2     |
| C(53)-C(52)-H(52A)  | 111.2     |
| C(51)-C(52)-H(52B)  | 111.2     |

|                     |       |
|---------------------|-------|
| C(53)-C(52)-H(52B)  | 111.2 |
| H(52A)-C(52)-H(52B) | 109.1 |

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Symmetry transformations used to generate equivalent atoms:

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

|       | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|-------|----------|----------|----------|----------|----------|----------|
| Ru(1) | 14(1)    | 20(1)    | 28(1)    | -1(1)    | 1(1)     | 0(1)     |
| Cl(1) | 24(1)    | 32(1)    | 36(1)    | -5(1)    | 3(1)     | 4(1)     |
| P(1)  | 16(1)    | 20(1)    | 29(1)    | 0(1)     | 2(1)     | 0(1)     |
| P(2)  | 17(1)    | 21(1)    | 27(1)    | -1(1)    | 2(1)     | 0(1)     |
| N(1)  | 15(2)    | 23(3)    | 30(2)    | 1(2)     | -1(2)    | -6(2)    |
| O(1)  | 18(2)    | 21(2)    | 28(2)    | -2(2)    | 0(2)     | -1(2)    |
| O(2)  | 39(3)    | 30(3)    | 44(3)    | 8(2)     | -5(2)    | -2(2)    |
| C(50) | 33(4)    | 22(3)    | 33(3)    | 4(3)     | -4(3)    | 11(3)    |
| O(4)  | 27(3)    | 43(3)    | 62(3)    | 10(2)    | -3(2)    | -4(2)    |
| C(1)  | 16(3)    | 23(3)    | 30(3)    | 3(2)     | 2(2)     | 1(2)     |
| C(2)  | 23(3)    | 24(3)    | 35(3)    | 0(3)     | 0(2)     | 3(2)     |
| C(3)  | 30(3)    | 38(4)    | 33(3)    | -8(3)    | 6(3)     | 9(3)     |
| C(4)  | 22(3)    | 62(5)    | 31(3)    | 2(3)     | 4(3)     | 18(3)    |
| C(5)  | 25(3)    | 39(4)    | 39(3)    | 5(3)     | 2(3)     | -3(3)    |
| O(3)  | 104(6)   | 83(6)    | 104(6)   | 28(5)    | 4(5)     | 21(5)    |
| C(6)  | 18(3)    | 26(3)    | 39(3)    | 1(3)     | 1(2)     | -1(2)    |
| C(7)  | 22(3)    | 31(3)    | 29(3)    | 0(3)     | 1(2)     | -1(3)    |
| C(8)  | 20(3)    | 42(4)    | 34(3)    | 2(3)     | 4(2)     | -2(3)    |
| C(9)  | 26(3)    | 59(5)    | 41(4)    | 4(3)     | 8(3)     | -7(3)    |
| C(10) | 47(4)    | 46(5)    | 45(4)    | 8(3)     | 11(3)    | -10(4)   |
| C(11) | 46(4)    | 36(4)    | 52(4)    | 13(3)    | 13(3)    | 0(3)     |
| C(12) | 23(3)    | 32(4)    | 50(4)    | 8(3)     | 9(3)     | 4(3)     |
| C(13) | 22(3)    | 25(3)    | 32(3)    | -6(3)    | 3(2)     | -1(2)    |
| C(14) | 50(4)    | 31(4)    | 39(4)    | -4(3)    | -1(3)    | 5(3)     |
| C(15) | 48(4)    | 55(5)    | 32(4)    | -4(3)    | -7(3)    | 9(4)     |
| C(16) | 36(4)    | 43(4)    | 35(3)    | -16(3)   | 2(3)     | -4(3)    |
| C(17) | 38(4)    | 28(4)    | 53(4)    | -11(3)   | -1(3)    | 2(3)     |
| C(18) | 25(3)    | 27(4)    | 47(4)    | -4(3)    | -3(3)    | 4(3)     |
| C(19) | 20(3)    | 28(3)    | 32(3)    | 2(3)     | -1(2)    | 5(3)     |
| C(20) | 49(4)    | 35(4)    | 28(3)    | 1(3)     | 3(3)     | 5(3)     |
| C(21) | 57(5)    | 41(4)    | 31(3)    | -6(3)    | -4(3)    | 16(4)    |

|       |         |         |         |        |         |        |
|-------|---------|---------|---------|--------|---------|--------|
| C(22) | 29(4)   | 70(6)   | 41(4)   | -8(4)  | 8(3)    | 10(4)  |
| C(23) | 28(4)   | 76(6)   | 46(4)   | -5(4)  | 15(3)   | -13(4) |
| C(24) | 24(3)   | 38(4)   | 45(4)   | -9(3)  | 2(3)    | -6(3)  |
| C(25) | 21(3)   | 24(3)   | 37(3)   | 6(3)   | -3(3)   | -2(3)  |
| C(26) | 24(3)   | 33(4)   | 38(3)   | 0(3)   | -2(3)   | -3(3)  |
| C(27) | 23(3)   | 42(4)   | 52(4)   | 5(3)   | 3(3)    | -2(3)  |
| C(28) | 24(3)   | 56(5)   | 58(5)   | 10(4)  | -5(3)   | -10(3) |
| C(29) | 36(4)   | 74(6)   | 41(4)   | -1(4)  | -11(3)  | -18(4) |
| C(30) | 34(4)   | 50(5)   | 30(3)   | -1(3)  | -3(3)   | -8(3)  |
| C(31) | 17(3)   | 25(3)   | 35(3)   | 1(2)   | 6(2)    | 4(2)   |
| C(32) | 39(4)   | 27(3)   | 38(4)   | 0(3)   | -9(3)   | 3(3)   |
| C(33) | 43(4)   | 35(4)   | 43(4)   | 8(3)   | -9(3)   | 6(3)   |
| C(34) | 44(4)   | 14(3)   | 56(4)   | 2(3)   | -3(3)   | 2(3)   |
| C(35) | 27(3)   | 33(4)   | 39(3)   | -6(3)  | 2(3)    | -8(3)  |
| C(36) | 24(3)   | 23(3)   | 35(3)   | -1(3)  | 1(2)    | 4(2)   |
| C(37) | 18(3)   | 35(4)   | 31(3)   | 1(3)   | 6(2)    | 3(3)   |
| C(38) | 22(3)   | 34(4)   | 39(3)   | -4(3)  | 5(3)    | 10(3)  |
| C(39) | 26(3)   | 21(3)   | 35(3)   | 0(3)   | 1(2)    | 4(3)   |
| C(40) | 16(3)   | 24(3)   | 30(3)   | 1(2)   | 2(2)    | -1(2)  |
| C(41) | 18(3)   | 24(3)   | 29(3)   | 1(2)   | -2(2)   | 1(2)   |
| C(42) | 15(3)   | 21(3)   | 35(3)   | -6(2)  | 5(2)    | -4(2)  |
| C(43) | 25(3)   | 29(3)   | 36(3)   | -4(3)  | 5(3)    | -2(3)  |
| C(44) | 57(5)   | 33(4)   | 68(5)   | 18(4)  | -5(4)   | 5(4)   |
| C(45) | 41(4)   | 26(4)   | 46(4)   | -2(3)  | 13(3)   | -11(3) |
| C(46) | 29(4)   | 39(4)   | 52(4)   | -15(3) | 13(3)   | -13(3) |
| C(47) | 19(3)   | 53(5)   | 40(4)   | -12(3) | 2(3)    | -3(3)  |
| C(48) | 20(3)   | 31(4)   | 36(3)   | -6(3)  | 1(2)    | -2(3)  |
| C(54) | 134(13) | 77(9)   | 154(13) | 8(9)   | -53(11) | -30(9) |
| C(53) | 70(10)  | 107(12) | 310(30) | 32(15) | -12(14) | 22(9)  |
| C(51) | 168(17) | 152(16) | 125(13) | 65(12) | 46(12)  | 19(13) |
| C(52) | 180(20) | 240(30) | 240(30) | 10(20) | 140(20) | 80(20) |

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Table 5. Hydrogen coordinates (  $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for 3.

|       | x     | y     | z     | U(eq) |
|-------|-------|-------|-------|-------|
| H(2)  | 7802  | 10494 | 7675  | 33    |
| H(3)  | 5856  | 11015 | 7875  | 40    |
| H(4)  | 3972  | 10292 | 7818  | 45    |
| H(5)  | 4018  | 9026  | 7592  | 41    |
| H(6)  | 5932  | 8505  | 7349  | 34    |
| H(8)  | 11262 | 9129  | 7216  | 38    |
| H(9)  | 12585 | 10001 | 6861  | 50    |
| H(10) | 11674 | 11095 | 6472  | 55    |
| H(11) | 9450  | 11310 | 6429  | 53    |
| H(12) | 8108  | 10459 | 6784  | 42    |
| H(14) | 7138  | 9268  | 6323  | 49    |
| H(15) | 6133  | 8543  | 5642  | 55    |
| H(16) | 6336  | 7240  | 5667  | 46    |
| H(17) | 7500  | 6657  | 6373  | 48    |
| H(18) | 8524  | 7382  | 7062  | 41    |
| H(20) | 10374 | 9117  | 9487  | 45    |
| H(21) | 9221  | 9467  | 10155 | 53    |
| H(22) | 7913  | 8584  | 10512 | 56    |
| H(23) | 7829  | 7354  | 10210 | 59    |
| H(24) | 8979  | 7000  | 9546  | 43    |
| H(26) | 12908 | 7824  | 8370  | 39    |
| H(27) | 15125 | 8054  | 8579  | 47    |
| H(28) | 15976 | 8399  | 9415  | 56    |
| H(29) | 14598 | 8521  | 10045 | 62    |
| H(30) | 12355 | 8275  | 9841  | 46    |
| H(32) | 11788 | 6710  | 9652  | 43    |
| H(33) | 11802 | 5415  | 9759  | 50    |
| H(34) | 10687 | 4639  | 9114  | 47    |
| H(35) | 9659  | 5165  | 8359  | 40    |
| H(36) | 9691  | 6480  | 8241  | 33    |

|        |       |       |       |     |
|--------|-------|-------|-------|-----|
| H(37)  | 7092  | 9031  | 8734  | 33  |
| H(38)  | 7289  | 10322 | 9129  | 38  |
| H(39)  | 9416  | 10867 | 8960  | 34  |
| H(44A) | 11268 | 12096 | 7606  | 81  |
| H(44B) | 10588 | 12356 | 8084  | 81  |
| H(44C) | 9735  | 12025 | 7587  | 81  |
| H(45)  | 12840 | 12089 | 8314  | 44  |
| H(46)  | 14712 | 11732 | 8857  | 47  |
| H(47)  | 14927 | 10519 | 9187  | 45  |
| H(48)  | 13235 | 9646  | 8978  | 35  |
| H(54A) | 3547  | 3543  | 10417 | 154 |
| H(54B) | 3811  | 4422  | 10383 | 154 |
| H(53A) | 5511  | 3389  | 10321 | 197 |
| H(53B) | 5661  | 4245  | 10157 | 197 |
| H(51A) | 3788  | 4349  | 9143  | 175 |
| H(51B) | 3208  | 3520  | 9070  | 175 |
| H(52A) | 5657  | 3772  | 9348  | 254 |
| H(52B) | 4971  | 3008  | 9488  | 254 |

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|                                   |                                                                  |                 |
|-----------------------------------|------------------------------------------------------------------|-----------------|
| Table 1 Identification code       | 4                                                                |                 |
| Empirical formula                 | C <sub>23</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub> Ru |                 |
| Formula weight                    | 477.51                                                           |                 |
| Temperature                       | 150(2) K                                                         |                 |
| Wavelength                        | 0.71073 Å                                                        |                 |
| Crystal system                    | Monoclinic                                                       |                 |
| Space group                       | P2 <sub>1</sub> /c                                               |                 |
| Unit cell dimensions              | a = 10.157(5) Å                                                  | α = 90°.        |
|                                   | b = 15.836(7) Å                                                  | β = 105.44(3)°. |
|                                   | c = 14.019(8) Å                                                  | γ = 90°.        |
| Volume                            | 2173.5(19) Å <sup>3</sup>                                        |                 |
| Z                                 | 4                                                                |                 |
| Density (calculated)              | 1.465 Mg/m <sup>3</sup>                                          |                 |
| Absorption coefficient            | 0.748 mm <sup>-1</sup>                                           |                 |
| F(000)                            | 980                                                              |                 |
| Crystal size                      | 0.180 x 0.140 x 0.120 mm <sup>3</sup>                            |                 |
| Theta range for data collection   | 1.981 to 28.281°.                                                |                 |
| Index ranges                      | -13 ≤ h ≤ 13, -21 ≤ k ≤ 21, -18 ≤ l ≤ 13                         |                 |
| Reflections collected             | 26439                                                            |                 |
| Independent reflections           | 5380 [R(int) = 0.0893]                                           |                 |
| Completeness to theta = 25.242°   | 99.9 %                                                           |                 |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                      |                 |
| Data / restraints / parameters    | 5380 / 0 / 266                                                   |                 |
| Goodness-of-fit on F <sup>2</sup> | 0.968                                                            |                 |
| Final R indices [I > 2σ(I)]       | R <sub>1</sub> = 0.0568, wR <sub>2</sub> = 0.1449                |                 |
| R indices (all data)              | R <sub>1</sub> = 0.0890, wR <sub>2</sub> = 0.1724                |                 |
| Extinction coefficient            | n/a                                                              |                 |
| Largest diff. peak and hole       | 1.071 and -2.014 e.Å <sup>-3</sup>                               |                 |

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

|       | x        | y       | z        | U(eq) |
|-------|----------|---------|----------|-------|
| Ru(1) | -242(1)  | 8644(1) | 1100(1)  | 32(1) |
| O(1)  | -2459(4) | 8030(3) | -1937(3) | 69(1) |
| O(2)  | 1228(3)  | 8528(2) | 278(2)   | 38(1) |
| O(3)  | 3995(4)  | 6830(3) | 711(3)   | 59(1) |
| N(1)  | -1625(5) | 8455(3) | -262(3)  | 49(1) |
| C(23) | -2004(5) | 8230(3) | -1073(4) | 41(1) |
| N(2)  | 54(4)    | 7361(2) | 1070(3)  | 35(1) |
| C(18) | -562(6)  | 8665(3) | 2583(4)  | 40(1) |
| C(16) | 816(5)   | 8879(3) | 2655(4)  | 41(1) |
| C(14) | 1133(5)  | 9527(3) | 2076(4)  | 39(1) |
| C(15) | 56(5)    | 9984(2) | 1434(4)  | 37(1) |
| C(17) | -1298(4) | 9780(2) | 1352(4)  | 39(1) |
| C(19) | -1647(5) | 9111(3) | 1941(4)  | 42(1) |
| C(20) | -3115(6) | 8894(3) | 1919(5)  | 57(2) |
| C(22) | -3445(7) | 9338(4) | 2821(6)  | 85(2) |
| C(21) | -4146(6) | 9132(4) | 964(5)   | 82(2) |
| C(13) | 2600(5)  | 9704(3) | 2079(5)  | 59(2) |
| C(5)  | 1580(4)  | 7776(2) | 124(3)   | 33(1) |
| C(6)  | 2545(5)  | 7677(2) | -487(3)  | 34(1) |
| C(11) | 3748(5)  | 7201(3) | -202(4)  | 43(1) |
| C(12) | 5164(8)  | 6315(4) | 1035(5)  | 79(2) |
| C(10) | 4610(6)  | 7150(3) | -828(4)  | 55(1) |
| C(9)  | 4314(6)  | 7568(3) | -1725(4) | 56(1) |
| C(8)  | 3120(6)  | 8041(3) | -2025(4) | 49(1) |
| C(7)  | 2264(5)  | 8099(3) | -1403(4) | 39(1) |
| C(4)  | 950(5)   | 7115(2) | 514(4)   | 37(1) |
| C(1)  | -473(5)  | 6665(3) | 1352(4)  | 44(1) |
| C(2)  | 80(6)    | 5959(3) | 995(4)   | 52(1) |
| C(3)  | 961(6)   | 6234(3) | 465(4)   | 47(1) |

Table 3 4.

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|              |          |
|--------------|----------|
| Ru(1)-N(2)   | 2.057(3) |
| Ru(1)-N(1)   | 2.070(5) |
| Ru(1)-O(2)   | 2.124(3) |
| Ru(1)-C(17)  | 2.171(4) |
| Ru(1)-C(15)  | 2.177(4) |
| Ru(1)-C(14)  | 2.181(4) |
| Ru(1)-C(18)  | 2.188(5) |
| Ru(1)-C(16)  | 2.189(5) |
| Ru(1)-C(19)  | 2.206(5) |
| O(1)-C(23)   | 1.218(6) |
| O(2)-C(5)    | 1.278(5) |
| O(3)-C(11)   | 1.370(6) |
| O(3)-C(12)   | 1.412(7) |
| N(1)-C(23)   | 1.155(6) |
| N(2)-C(1)    | 1.330(6) |
| N(2)-C(4)    | 1.401(6) |
| C(18)-C(19)  | 1.412(7) |
| C(18)-C(16)  | 1.417(8) |
| C(18)-H(18)  | 0.9300   |
| C(16)-C(14)  | 1.398(7) |
| C(16)-H(16)  | 0.9300   |
| C(14)-C(15)  | 1.417(6) |
| C(14)-C(13)  | 1.515(6) |
| C(15)-C(17)  | 1.388(6) |
| C(15)-H(15)  | 0.9300   |
| C(17)-C(19)  | 1.445(6) |
| C(17)-H(17)  | 0.9300   |
| C(19)-C(20)  | 1.523(7) |
| C(20)-C(21)  | 1.512(8) |
| C(20)-C(22)  | 1.560(8) |
| C(20)-H(20)  | 0.9800   |
| C(22)-H(22A) | 0.9600   |
| C(22)-H(22B) | 0.9600   |
| C(22)-H(22C) | 0.9600   |

|                  |            |
|------------------|------------|
| C(21)-H(21A)     | 0.9600     |
| C(21)-H(21B)     | 0.9600     |
| C(21)-H(21C)     | 0.9600     |
| C(13)-H(13A)     | 0.9600     |
| C(13)-H(13B)     | 0.9600     |
| C(13)-H(13C)     | 0.9600     |
| C(5)-C(4)        | 1.411(6)   |
| C(5)-C(6)        | 1.472(6)   |
| C(6)-C(11)       | 1.401(6)   |
| C(6)-C(7)        | 1.408(6)   |
| C(11)-C(10)      | 1.397(7)   |
| C(12)-H(12A)     | 0.9600     |
| C(12)-H(12B)     | 0.9600     |
| C(12)-H(12C)     | 0.9600     |
| C(10)-C(9)       | 1.382(8)   |
| C(10)-H(10)      | 0.9300     |
| C(9)-C(8)        | 1.391(7)   |
| C(9)-H(9)        | 0.9300     |
| C(8)-C(7)        | 1.389(7)   |
| C(8)-H(8)        | 0.9300     |
| C(7)-H(7)        | 0.9300     |
| C(4)-C(3)        | 1.398(6)   |
| C(1)-C(2)        | 1.401(8)   |
| C(1)-H(1)        | 0.9300     |
| C(2)-C(3)        | 1.377(8)   |
| C(2)-H(2)        | 0.9300     |
| C(3)-H(3)        | 0.9300     |
|                  |            |
| N(2)-Ru(1)-N(1)  | 84.53(16)  |
| N(2)-Ru(1)-O(2)  | 77.03(13)  |
| N(1)-Ru(1)-O(2)  | 83.61(16)  |
| N(2)-Ru(1)-C(17) | 154.61(16) |
| N(1)-Ru(1)-C(17) | 91.52(17)  |
| O(2)-Ru(1)-C(17) | 127.54(15) |
| N(2)-Ru(1)-C(15) | 162.79(18) |
| N(1)-Ru(1)-C(15) | 111.15(17) |

|                   |            |
|-------------------|------------|
| O(2)-Ru(1)-C(15)  | 97.09(14)  |
| C(17)-Ru(1)-C(15) | 37.22(16)  |
| N(2)-Ru(1)-C(14)  | 125.00(17) |
| N(1)-Ru(1)-C(14)  | 146.67(17) |
| O(2)-Ru(1)-C(14)  | 88.32(15)  |
| C(17)-Ru(1)-C(14) | 68.21(17)  |
| C(15)-Ru(1)-C(14) | 37.95(17)  |
| N(2)-Ru(1)-C(18)  | 95.40(15)  |
| N(1)-Ru(1)-C(18)  | 130.0(2)   |
| O(2)-Ru(1)-C(18)  | 145.20(18) |
| C(17)-Ru(1)-C(18) | 68.17(18)  |
| C(15)-Ru(1)-C(18) | 80.13(17)  |
| C(14)-Ru(1)-C(18) | 68.10(18)  |
| N(2)-Ru(1)-C(16)  | 98.77(17)  |
| N(1)-Ru(1)-C(16)  | 167.36(18) |
| O(2)-Ru(1)-C(16)  | 109.01(17) |
| C(17)-Ru(1)-C(16) | 80.25(18)  |
| C(15)-Ru(1)-C(16) | 67.53(18)  |
| C(14)-Ru(1)-C(16) | 37.32(18)  |
| C(18)-Ru(1)-C(16) | 37.8(2)    |
| N(2)-Ru(1)-C(19)  | 117.43(16) |
| N(1)-Ru(1)-C(19)  | 99.47(19)  |
| O(2)-Ru(1)-C(19)  | 165.35(13) |
| C(17)-Ru(1)-C(19) | 38.54(17)  |
| C(15)-Ru(1)-C(19) | 68.39(16)  |
| C(14)-Ru(1)-C(19) | 81.26(18)  |
| C(18)-Ru(1)-C(19) | 37.49(18)  |
| C(16)-Ru(1)-C(19) | 68.13(19)  |
| C(5)-O(2)-Ru(1)   | 116.2(3)   |
| C(11)-O(3)-C(12)  | 118.5(5)   |
| C(23)-N(1)-Ru(1)  | 156.9(4)   |
| N(1)-C(23)-O(1)   | 176.3(6)   |
| C(1)-N(2)-C(4)    | 107.9(4)   |
| C(1)-N(2)-Ru(1)   | 137.8(3)   |
| C(4)-N(2)-Ru(1)   | 113.9(3)   |
| C(19)-C(18)-C(16) | 121.0(4)   |



|                   |          |
|-------------------|----------|
| C(19)-C(18)-Ru(1) | 71.9(3)  |
| C(16)-C(18)-Ru(1) | 71.2(3)  |
| C(19)-C(18)-H(18) | 119.5    |
| C(16)-C(18)-H(18) | 119.5    |
| Ru(1)-C(18)-H(18) | 130.0    |
| C(14)-C(16)-C(18) | 120.6(4) |
| C(14)-C(16)-Ru(1) | 71.0(3)  |
| C(18)-C(16)-Ru(1) | 71.0(3)  |
| C(14)-C(16)-H(16) | 119.7    |
| C(18)-C(16)-H(16) | 119.7    |
| Ru(1)-C(16)-H(16) | 131.0    |
| C(16)-C(14)-C(15) | 119.1(4) |
| C(16)-C(14)-C(13) | 120.9(4) |
| C(15)-C(14)-C(13) | 119.9(4) |
| C(16)-C(14)-Ru(1) | 71.7(3)  |
| C(15)-C(14)-Ru(1) | 70.9(3)  |
| C(13)-C(14)-Ru(1) | 125.8(3) |
| C(17)-C(15)-C(14) | 120.9(4) |
| C(17)-C(15)-Ru(1) | 71.1(2)  |
| C(14)-C(15)-Ru(1) | 71.2(2)  |
| C(17)-C(15)-H(15) | 119.5    |
| C(14)-C(15)-H(15) | 119.5    |
| Ru(1)-C(15)-H(15) | 130.9    |
| C(15)-C(17)-C(19) | 120.8(4) |
| C(15)-C(17)-Ru(1) | 71.6(2)  |
| C(19)-C(17)-Ru(1) | 72.0(2)  |
| C(15)-C(17)-H(17) | 119.6    |
| C(19)-C(17)-H(17) | 119.6    |
| Ru(1)-C(17)-H(17) | 129.2    |
| C(18)-C(19)-C(17) | 117.5(4) |
| C(18)-C(19)-C(20) | 119.6(5) |
| C(17)-C(19)-C(20) | 122.8(5) |
| C(18)-C(19)-Ru(1) | 70.6(3)  |
| C(17)-C(19)-Ru(1) | 69.4(2)  |
| C(20)-C(19)-Ru(1) | 133.1(4) |
| C(21)-C(20)-C(19) | 113.9(5) |

|                     |          |
|---------------------|----------|
| C(21)-C(20)-C(22)   | 111.0(5) |
| C(19)-C(20)-C(22)   | 107.6(5) |
| C(21)-C(20)-H(20)   | 108.1    |
| C(19)-C(20)-H(20)   | 108.1    |
| C(22)-C(20)-H(20)   | 108.1    |
| C(20)-C(22)-H(22A)  | 109.5    |
| C(20)-C(22)-H(22B)  | 109.5    |
| H(22A)-C(22)-H(22B) | 109.5    |
| C(20)-C(22)-H(22C)  | 109.5    |
| H(22A)-C(22)-H(22C) | 109.5    |
| H(22B)-C(22)-H(22C) | 109.5    |
| C(20)-C(21)-H(21A)  | 109.5    |
| C(20)-C(21)-H(21B)  | 109.5    |
| H(21A)-C(21)-H(21B) | 109.5    |
| C(20)-C(21)-H(21C)  | 109.5    |
| H(21A)-C(21)-H(21C) | 109.5    |
| H(21B)-C(21)-H(21C) | 109.5    |
| C(14)-C(13)-H(13A)  | 109.5    |
| C(14)-C(13)-H(13B)  | 109.5    |
| H(13A)-C(13)-H(13B) | 109.5    |
| C(14)-C(13)-H(13C)  | 109.5    |
| H(13A)-C(13)-H(13C) | 109.5    |
| H(13B)-C(13)-H(13C) | 109.5    |
| O(2)-C(5)-C(4)      | 116.7(4) |
| O(2)-C(5)-C(6)      | 117.2(4) |
| C(4)-C(5)-C(6)      | 126.0(4) |
| C(11)-C(6)-C(7)     | 117.7(4) |
| C(11)-C(6)-C(5)     | 123.9(4) |
| C(7)-C(6)-C(5)      | 118.4(4) |
| O(3)-C(11)-C(10)    | 125.0(4) |
| O(3)-C(11)-C(6)     | 115.2(4) |
| C(10)-C(11)-C(6)    | 119.8(5) |
| O(3)-C(12)-H(12A)   | 109.5    |
| O(3)-C(12)-H(12B)   | 109.5    |
| H(12A)-C(12)-H(12B) | 109.5    |
| O(3)-C(12)-H(12C)   | 109.5    |

|                     |          |
|---------------------|----------|
| H(12A)-C(12)-H(12C) | 109.5    |
| H(12B)-C(12)-H(12C) | 109.5    |
| C(9)-C(10)-C(11)    | 121.5(5) |
| C(9)-C(10)-H(10)    | 119.3    |
| C(11)-C(10)-H(10)   | 119.3    |
| C(10)-C(9)-C(8)     | 119.6(5) |
| C(10)-C(9)-H(9)     | 120.2    |
| C(8)-C(9)-H(9)      | 120.2    |
| C(7)-C(8)-C(9)      | 119.1(5) |
| C(7)-C(8)-H(8)      | 120.4    |
| C(9)-C(8)-H(8)      | 120.4    |
| C(8)-C(7)-C(6)      | 122.1(4) |
| C(8)-C(7)-H(7)      | 118.9    |
| C(6)-C(7)-H(7)      | 118.9    |
| C(3)-C(4)-N(2)      | 108.7(4) |
| C(3)-C(4)-C(5)      | 135.3(5) |
| N(2)-C(4)-C(5)      | 116.0(4) |
| N(2)-C(1)-C(2)      | 108.9(5) |
| N(2)-C(1)-H(1)      | 125.5    |
| C(2)-C(1)-H(1)      | 125.5    |
| C(3)-C(2)-C(1)      | 108.7(4) |
| C(3)-C(2)-H(2)      | 125.6    |
| C(1)-C(2)-H(2)      | 125.6    |
| C(2)-C(3)-C(4)      | 105.8(5) |
| C(2)-C(3)-H(3)      | 127.1    |
| C(4)-C(3)-H(3)      | 127.1    |

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Symmetry transformations used to generate equivalent atoms:

Table 4 ( $\text{\AA}^2 \times 10^3$ ) for 4. The anisotropicdisplacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$ 

|       | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|-------|----------|----------|----------|----------|----------|----------|
| Ru(1) | 36(1)    | 22(1)    | 39(1)    | 1(1)     | 11(1)    | 2(1)     |
| O(1)  | 70(3)    | 75(3)    | 58(3)    | -23(2)   | 11(2)    | -4(2)    |
| O(2)  | 47(2)    | 24(1)    | 46(2)    | 0(1)     | 18(2)    | 2(1)     |
| O(3)  | 52(2)    | 75(3)    | 49(2)    | 13(2)    | 12(2)    | 27(2)    |
| N(1)  | 51(3)    | 45(2)    | 48(3)    | -3(2)    | 8(2)     | 5(2)     |
| C(23) | 34(3)    | 34(2)    | 54(3)    | -3(2)    | 11(2)    | 0(2)     |
| N(2)  | 43(2)    | 20(2)    | 44(2)    | 2(2)     | 12(2)    | 3(1)     |
| C(18) | 62(3)    | 27(2)    | 37(3)    | -2(2)    | 21(2)    | -1(2)    |
| C(16) | 48(3)    | 36(2)    | 35(3)    | -6(2)    | 7(2)     | 7(2)     |
| C(14) | 40(3)    | 31(2)    | 47(3)    | -8(2)    | 11(2)    | -2(2)    |
| C(15) | 45(3)    | 21(2)    | 46(3)    | -3(2)    | 15(2)    | 1(2)     |
| C(17) | 40(3)    | 24(2)    | 54(3)    | -1(2)    | 14(2)    | 7(2)     |
| C(19) | 47(3)    | 30(2)    | 55(3)    | -7(2)    | 26(2)    | 0(2)     |
| C(20) | 47(3)    | 44(3)    | 88(5)    | -2(3)    | 33(3)    | -1(2)    |
| C(22) | 76(5)    | 87(5)    | 113(6)   | -8(4)    | 62(4)    | -9(4)    |
| C(21) | 46(3)    | 89(5)    | 107(6)   | -12(4)   | 14(4)    | -5(3)    |
| C(13) | 39(3)    | 49(3)    | 82(4)    | -6(3)    | 2(3)     | -6(2)    |
| C(5)  | 32(2)    | 28(2)    | 36(2)    | -2(2)    | 2(2)     | 3(2)     |
| C(6)  | 38(2)    | 26(2)    | 40(3)    | -7(2)    | 12(2)    | -1(2)    |
| C(11) | 45(3)    | 42(2)    | 45(3)    | -3(2)    | 15(2)    | 11(2)    |
| C(12) | 80(4)    | 85(5)    | 66(5)    | 12(3)    | 8(4)     | 44(4)    |
| C(10) | 53(3)    | 57(3)    | 57(4)    | -1(3)    | 19(3)    | 15(3)    |
| C(9)  | 57(3)    | 56(3)    | 63(4)    | -8(3)    | 31(3)    | -1(3)    |
| C(8)  | 67(3)    | 36(2)    | 48(3)    | 3(2)     | 22(3)    | -3(2)    |
| C(7)  | 47(3)    | 27(2)    | 43(3)    | -1(2)    | 13(2)    | 2(2)     |
| C(4)  | 45(3)    | 24(2)    | 43(3)    | -3(2)    | 12(2)    | 3(2)     |
| C(1)  | 55(3)    | 29(2)    | 53(3)    | 0(2)     | 20(3)    | -8(2)    |
| C(2)  | 73(4)    | 24(2)    | 62(4)    | 0(2)     | 23(3)    | -8(2)    |
| C(3)  | 65(4)    | 27(2)    | 51(3)    | -6(2)    | 16(3)    | 4(2)     |

Table 5 displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for 4.

|        | x     | y     | z     | U(eq) |
|--------|-------|-------|-------|-------|
| H(18)  | -755  | 8226  | 2964  | 49    |
| H(16)  | 1516  | 8585  | 3091  | 49    |
| H(15)  | 260   | 10428 | 1062  | 44    |
| H(17)  | -1990 | 10078 | 913   | 47    |
| H(20)  | -3171 | 8282  | 2009  | 69    |
| H(22A) | -3320 | 9937  | 2778  | 128   |
| H(22B) | -2845 | 9128  | 3423  | 128   |
| H(22C) | -4375 | 9224  | 2817  | 128   |
| H(21A) | -3916 | 8856  | 419   | 123   |
| H(21B) | -4135 | 9733  | 874   | 123   |
| H(21C) | -5041 | 8958  | 991   | 123   |
| H(13A) | 3163  | 9233  | 2365  | 89    |
| H(13B) | 2913  | 10203 | 2461  | 89    |
| H(13C) | 2653  | 9788  | 1412  | 89    |
| H(12A) | 5968  | 6644  | 1066  | 119   |
| H(12B) | 5115  | 5856  | 580   | 119   |
| H(12C) | 5203  | 6095  | 1681  | 119   |
| H(10)  | 5402  | 6827  | -636  | 66    |
| H(9)   | 4909  | 7534  | -2126 | 67    |
| H(8)   | 2898  | 8314  | -2634 | 59    |
| H(7)   | 1480  | 8429  | -1598 | 47    |
| H(1)   | -1105 | 6649  | 1725  | 53    |
| H(2)   | -116  | 5399  | 1099  | 63    |
| H(3)   | 1461  | 5901  | 140   | 57    |

Table 1. Crystal data and structure refinement for 5.

|                                   |                                                                  |                  |
|-----------------------------------|------------------------------------------------------------------|------------------|
| Identification code               | 5                                                                |                  |
| Empirical formula                 | C <sub>22</sub> H <sub>24</sub> N <sub>4</sub> O <sub>2</sub> Ru |                  |
| Formula weight                    | 477.52                                                           |                  |
| Temperature                       | 150 K                                                            |                  |
| Wavelength                        | 0.71073 Å                                                        |                  |
| Crystal system                    | Monoclinic                                                       |                  |
| Space group                       | P2(1)/c                                                          |                  |
| Unit cell dimensions              | a = 17.3849(14) Å                                                | α = 90°.         |
|                                   | b = 9.2423(7) Å                                                  | β = 112.379(4)°. |
|                                   | c = 13.8157(11) Å                                                | γ = 90°.         |
| Volume                            | 2052.7(3) Å <sup>3</sup>                                         |                  |
| Z                                 | 4                                                                |                  |
| Density (calculated)              | 1.545 Mg/m <sup>3</sup>                                          |                  |
| Absorption coefficient            | 0.787 mm <sup>-1</sup>                                           |                  |
| F(000)                            | 976.0                                                            |                  |
| Crystal size                      | 0.18 x 0.14 x 0.12 mm <sup>3</sup>                               |                  |
| Theta range for data collection   | 2.54 to 28.74°.                                                  |                  |
| Index ranges                      | -19 ≤ h ≤ 23, -12 ≤ k ≤ 12, -18 ≤ l ≤ 18                         |                  |
| Reflections collected             | 18124                                                            |                  |
| Independent reflections           | 5243 [R(int) = 0.0298]                                           |                  |
| Completeness to theta = 28.74°    | 98.2 %                                                           |                  |
| Absorption correction             | Semi-empirical from equivalents                                  |                  |
| Max. and min. transmission        | 0.9196 and 0.8828                                                |                  |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                      |                  |
| Data / restraints / parameters    | 5243 / 0 / 266                                                   |                  |
| Goodness-of-fit on F <sup>2</sup> | 1.067                                                            |                  |
| Final R indices [I > 2σ(I)]       | R1 = 0.0306, wR2 = 0.0783                                        |                  |
| R indices (all data)              | R1 = 0.0356, wR2 = 0.0810                                        |                  |
| Largest diff. peak and hole       | 0.870 and -0.699 e.Å <sup>-3</sup>                               |                  |

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 5.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

|       | x       | y        | z       | $U(\text{eq})$ |
|-------|---------|----------|---------|----------------|
| Ru(1) | 6689(1) | 5397(1)  | 6571(1) | 19(1)          |
| O(1)  | 7318(1) | 6250(2)  | 5659(1) | 24(1)          |
| O(2)  | 8546(1) | 8655(2)  | 5937(2) | 36(1)          |
| N(1)  | 6348(1) | 3654(2)  | 5506(2) | 29(1)          |
| N(2)  | 6820(1) | 3212(2)  | 5126(2) | 26(1)          |
| N(3)  | 7246(2) | 2740(3)  | 4733(2) | 38(1)          |
| N(4)  | 7841(1) | 4419(2)  | 7204(2) | 20(1)          |
| C(1)  | 5652(1) | 6952(2)  | 6162(2) | 24(1)          |
| C(2)  | 6391(2) | 7600(3)  | 6879(2) | 27(1)          |
| C(3)  | 6832(2) | 6891(3)  | 7844(2) | 32(1)          |
| C(4)  | 6559(2) | 5527(3)  | 8049(2) | 35(1)          |
| C(5)  | 5835(2) | 4870(3)  | 7345(2) | 32(1)          |
| C(6)  | 5546(2) | 3417(3)  | 7555(3) | 57(1)          |
| C(7)  | 5386(2) | 5614(2)  | 6395(2) | 27(1)          |
| C(8)  | 6730(2) | 9004(3)  | 6631(3) | 40(1)          |
| C(9)  | 6542(3) | 10221(3) | 7269(4) | 63(1)          |
| C(10) | 6401(3) | 9384(3)  | 5480(3) | 55(1)          |
| C(11) | 8390(1) | 4835(2)  | 6742(2) | 21(1)          |
| C(12) | 9150(2) | 4099(3)  | 7234(2) | 26(1)          |
| C(13) | 9048(2) | 3225(3)  | 7990(2) | 28(1)          |
| C(14) | 8233(2) | 3452(2)  | 7945(2) | 24(1)          |
| C(15) | 8064(1) | 5806(2)  | 5909(2) | 22(1)          |
| C(16) | 8528(1) | 6327(2)  | 5262(2) | 24(1)          |
| C(17) | 8711(2) | 5367(3)  | 4610(2) | 32(1)          |
| C(18) | 9053(2) | 5854(3)  | 3907(2) | 39(1)          |
| C(19) | 9222(2) | 7313(3)  | 3880(2) | 37(1)          |
| C(20) | 9064(2) | 8288(3)  | 4537(2) | 30(1)          |
| C(21) | 8720(2) | 7803(3)  | 5243(2) | 25(1)          |
| C(22) | 8707(2) | 10173(3) | 5920(3) | 39(1)          |

Table 3. Bond lengths [Å] and angles [°] for 5.

|            |            |
|------------|------------|
| Ru(1)-N(4) | 2.0640(19) |
| Ru(1)-N(1) | 2.109(2)   |
| Ru(1)-O(1) | 2.1114(15) |
| Ru(1)-C(4) | 2.142(2)   |
| Ru(1)-C(3) | 2.174(2)   |
| Ru(1)-C(2) | 2.182(2)   |
| Ru(1)-C(5) | 2.189(2)   |
| Ru(1)-C(7) | 2.193(2)   |
| Ru(1)-C(1) | 2.205(2)   |
| O(1)-C(15) | 1.276(3)   |
| O(2)-C(21) | 1.361(3)   |
| O(2)-C(22) | 1.433(3)   |
| N(1)-N(2)  | 1.204(3)   |
| N(2)-N(3)  | 1.157(3)   |
| N(4)-C(14) | 1.335(3)   |
| N(4)-C(11) | 1.388(3)   |
| C(1)-C(7)  | 1.400(3)   |
| C(1)-C(2)  | 1.423(3)   |
| C(1)-H(1)  | 0.9300     |
| C(2)-C(3)  | 1.420(4)   |
| C(2)-C(8)  | 1.517(4)   |
| C(3)-C(4)  | 1.414(4)   |
| C(3)-H(3)  | 0.9300     |
| C(4)-C(5)  | 1.401(4)   |
| C(4)-H(4)  | 0.9300     |
| C(5)-C(7)  | 1.424(4)   |
| C(5)-C(6)  | 1.500(4)   |
| C(6)-H(6A) | 0.9600     |
| C(6)-H(6B) | 0.9600     |
| C(6)-H(6C) | 0.9600     |
| C(7)-H(7)  | 0.9300     |
| C(8)-C(10) | 1.512(5)   |
| C(8)-C(9)  | 1.538(4)   |
| C(8)-H(8)  | 0.9800     |



|                 |            |
|-----------------|------------|
| C(9)-H(9A)      | 0.9600     |
| C(9)-H(9B)      | 0.9600     |
| C(9)-H(9C)      | 0.9600     |
| C(10)-H(10A)    | 0.9600     |
| C(10)-H(10B)    | 0.9600     |
| C(10)-H(10C)    | 0.9600     |
| C(11)-C(15)     | 1.398(3)   |
| C(11)-C(12)     | 1.411(3)   |
| C(12)-C(13)     | 1.384(3)   |
| C(12)-H(12)     | 0.9300     |
| C(13)-C(14)     | 1.410(3)   |
| C(13)-H(13)     | 0.9300     |
| C(14)-H(14)     | 0.9300     |
| C(15)-C(16)     | 1.493(3)   |
| C(16)-C(17)     | 1.385(3)   |
| C(16)-C(21)     | 1.407(3)   |
| C(17)-C(18)     | 1.393(3)   |
| C(17)-H(17)     | 0.9300     |
| C(18)-C(19)     | 1.383(4)   |
| C(18)-H(18)     | 0.9300     |
| C(19)-C(20)     | 1.379(4)   |
| C(19)-H(19)     | 0.9300     |
| C(20)-C(21)     | 1.397(3)   |
| C(20)-H(20)     | 0.9300     |
| C(22)-H(22A)    | 0.9600     |
| C(22)-H(22B)    | 0.9600     |
| C(22)-H(22C)    | 0.9600     |
|                 |            |
| N(4)-Ru(1)-N(1) | 86.02(8)   |
| N(4)-Ru(1)-O(1) | 77.08(7)   |
| N(1)-Ru(1)-O(1) | 86.62(7)   |
| N(4)-Ru(1)-C(4) | 93.37(9)   |
| N(1)-Ru(1)-C(4) | 127.16(10) |
| O(1)-Ru(1)-C(4) | 144.61(10) |
| N(4)-Ru(1)-C(3) | 98.18(9)   |
| N(1)-Ru(1)-C(3) | 164.70(10) |

|                  |            |
|------------------|------------|
| O(1)-Ru(1)-C(3)  | 108.65(9)  |
| C(4)-Ru(1)-C(3)  | 38.24(11)  |
| N(4)-Ru(1)-C(2)  | 126.15(9)  |
| N(1)-Ru(1)-C(2)  | 145.50(9)  |
| O(1)-Ru(1)-C(2)  | 89.00(7)   |
| C(4)-Ru(1)-C(2)  | 69.10(10)  |
| C(3)-Ru(1)-C(2)  | 38.03(10)  |
| N(4)-Ru(1)-C(5)  | 115.15(9)  |
| N(1)-Ru(1)-C(5)  | 96.20(10)  |
| O(1)-Ru(1)-C(5)  | 167.56(8)  |
| C(4)-Ru(1)-C(5)  | 37.74(12)  |
| C(3)-Ru(1)-C(5)  | 68.67(11)  |
| C(2)-Ru(1)-C(5)  | 81.81(9)   |
| N(4)-Ru(1)-C(7)  | 151.88(8)  |
| N(1)-Ru(1)-C(7)  | 89.31(9)   |
| O(1)-Ru(1)-C(7)  | 130.34(8)  |
| C(4)-Ru(1)-C(7)  | 67.75(10)  |
| C(3)-Ru(1)-C(7)  | 80.04(10)  |
| C(2)-Ru(1)-C(7)  | 67.99(9)   |
| C(5)-Ru(1)-C(7)  | 37.92(10)  |
| N(4)-Ru(1)-C(1)  | 164.00(8)  |
| N(1)-Ru(1)-C(1)  | 109.49(9)  |
| O(1)-Ru(1)-C(1)  | 99.34(7)   |
| C(4)-Ru(1)-C(1)  | 80.51(9)   |
| C(3)-Ru(1)-C(1)  | 67.90(9)   |
| C(2)-Ru(1)-C(1)  | 37.84(9)   |
| C(5)-Ru(1)-C(1)  | 68.28(9)   |
| C(7)-Ru(1)-C(1)  | 37.12(8)   |
| C(15)-O(1)-Ru(1) | 114.97(14) |
| C(21)-O(2)-C(22) | 117.2(2)   |
| N(2)-N(1)-Ru(1)  | 120.43(17) |
| N(3)-N(2)-N(1)   | 176.7(3)   |
| C(14)-N(4)-C(11) | 107.37(19) |
| C(14)-N(4)-Ru(1) | 138.41(16) |
| C(11)-N(4)-Ru(1) | 114.21(14) |
| C(7)-C(1)-C(2)   | 120.1(2)   |

|                  |            |
|------------------|------------|
| C(7)-C(1)-Ru(1)  | 71.00(13)  |
| C(2)-C(1)-Ru(1)  | 70.21(13)  |
| C(7)-C(1)-H(1)   | 119.9      |
| C(2)-C(1)-H(1)   | 119.9      |
| Ru(1)-C(1)-H(1)  | 131.7      |
| C(3)-C(2)-C(1)   | 118.7(2)   |
| C(3)-C(2)-C(8)   | 119.3(2)   |
| C(1)-C(2)-C(8)   | 121.9(2)   |
| C(3)-C(2)-Ru(1)  | 70.68(14)  |
| C(1)-C(2)-Ru(1)  | 71.94(13)  |
| C(8)-C(2)-Ru(1)  | 127.83(16) |
| C(4)-C(3)-C(2)   | 119.9(2)   |
| C(4)-C(3)-Ru(1)  | 69.63(15)  |
| C(2)-C(3)-Ru(1)  | 71.29(13)  |
| C(4)-C(3)-H(3)   | 120.1      |
| C(2)-C(3)-H(3)   | 120.1      |
| Ru(1)-C(3)-H(3)  | 131.9      |
| C(5)-C(4)-C(3)   | 121.9(2)   |
| C(5)-C(4)-Ru(1)  | 72.96(15)  |
| C(3)-C(4)-Ru(1)  | 72.12(14)  |
| C(5)-C(4)-H(4)   | 119.1      |
| C(3)-C(4)-H(4)   | 119.1      |
| Ru(1)-C(4)-H(4)  | 128.1      |
| C(4)-C(5)-C(7)   | 117.6(2)   |
| C(4)-C(5)-C(6)   | 122.1(3)   |
| C(7)-C(5)-C(6)   | 120.2(3)   |
| C(4)-C(5)-Ru(1)  | 69.30(14)  |
| C(7)-C(5)-Ru(1)  | 71.21(13)  |
| C(6)-C(5)-Ru(1)  | 129.24(19) |
| C(5)-C(6)-H(6A)  | 109.5      |
| C(5)-C(6)-H(6B)  | 109.5      |
| H(6A)-C(6)-H(6B) | 109.5      |
| C(5)-C(6)-H(6C)  | 109.5      |
| H(6A)-C(6)-H(6C) | 109.5      |
| H(6B)-C(6)-H(6C) | 109.5      |
| C(1)-C(7)-C(5)   | 121.7(2)   |

|                     |            |
|---------------------|------------|
| C(1)-C(7)-Ru(1)     | 71.88(13)  |
| C(5)-C(7)-Ru(1)     | 70.88(13)  |
| C(1)-C(7)-H(7)      | 119.2      |
| C(5)-C(7)-H(7)      | 119.2      |
| Ru(1)-C(7)-H(7)     | 130.9      |
| C(10)-C(8)-C(2)     | 114.4(3)   |
| C(10)-C(8)-C(9)     | 110.8(3)   |
| C(2)-C(8)-C(9)      | 108.2(2)   |
| C(10)-C(8)-H(8)     | 107.8      |
| C(2)-C(8)-H(8)      | 107.8      |
| C(9)-C(8)-H(8)      | 107.8      |
| C(8)-C(9)-H(9A)     | 109.5      |
| C(8)-C(9)-H(9B)     | 109.5      |
| H(9A)-C(9)-H(9B)    | 109.5      |
| C(8)-C(9)-H(9C)     | 109.5      |
| H(9A)-C(9)-H(9C)    | 109.5      |
| H(9B)-C(9)-H(9C)    | 109.5      |
| C(8)-C(10)-H(10A)   | 109.5      |
| C(8)-C(10)-H(10B)   | 109.5      |
| H(10A)-C(10)-H(10B) | 109.5      |
| C(8)-C(10)-H(10C)   | 109.5      |
| H(10A)-C(10)-H(10C) | 109.5      |
| H(10B)-C(10)-H(10C) | 109.5      |
| N(4)-C(11)-C(15)    | 114.98(19) |
| N(4)-C(11)-C(12)    | 109.09(19) |
| C(15)-C(11)-C(12)   | 135.9(2)   |
| C(13)-C(12)-C(11)   | 106.2(2)   |
| C(13)-C(12)-H(12)   | 126.9      |
| C(11)-C(12)-H(12)   | 126.9      |
| C(12)-C(13)-C(14)   | 107.2(2)   |
| C(12)-C(13)-H(13)   | 126.4      |
| C(14)-C(13)-H(13)   | 126.4      |
| N(4)-C(14)-C(13)    | 110.1(2)   |
| N(4)-C(14)-H(14)    | 124.9      |
| C(13)-C(14)-H(14)   | 124.9      |
| O(1)-C(15)-C(11)    | 118.72(19) |

|                     |          |
|---------------------|----------|
| O(1)-C(15)-C(16)    | 117.3(2) |
| C(11)-C(15)-C(16)   | 123.9(2) |
| C(17)-C(16)-C(21)   | 119.6(2) |
| C(17)-C(16)-C(15)   | 119.5(2) |
| C(21)-C(16)-C(15)   | 120.7(2) |
| C(16)-C(17)-C(18)   | 120.7(2) |
| C(16)-C(17)-H(17)   | 119.6    |
| C(18)-C(17)-H(17)   | 119.6    |
| C(19)-C(18)-C(17)   | 119.1(2) |
| C(19)-C(18)-H(18)   | 120.5    |
| C(17)-C(18)-H(18)   | 120.5    |
| C(20)-C(19)-C(18)   | 121.4(2) |
| C(20)-C(19)-H(19)   | 119.3    |
| C(18)-C(19)-H(19)   | 119.3    |
| C(19)-C(20)-C(21)   | 119.7(2) |
| C(19)-C(20)-H(20)   | 120.1    |
| C(21)-C(20)-H(20)   | 120.1    |
| O(2)-C(21)-C(20)    | 125.1(2) |
| O(2)-C(21)-C(16)    | 115.4(2) |
| C(20)-C(21)-C(16)   | 119.5(2) |
| O(2)-C(22)-H(22A)   | 109.5    |
| O(2)-C(22)-H(22B)   | 109.5    |
| H(22A)-C(22)-H(22B) | 109.5    |
| O(2)-C(22)-H(22C)   | 109.5    |
| H(22A)-C(22)-H(22C) | 109.5    |
| H(22B)-C(22)-H(22C) | 109.5    |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 5. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

|       | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|-------|----------|----------|----------|----------|----------|----------|
| Ru(1) | 18(1)    | 20(1)    | 20(1)    | 1(1)     | 9(1)     | 3(1)     |
| O(1)  | 25(1)    | 24(1)    | 28(1)    | 4(1)     | 15(1)    | 4(1)     |
| O(2)  | 48(1)    | 23(1)    | 44(1)    | -5(1)    | 27(1)    | -6(1)    |
| N(1)  | 23(1)    | 31(1)    | 33(1)    | -8(1)    | 10(1)    | -1(1)    |
| N(2)  | 27(1)    | 22(1)    | 27(1)    | -2(1)    | 9(1)     | -1(1)    |
| N(3)  | 44(1)    | 34(1)    | 44(1)    | -10(1)   | 26(1)    | -1(1)    |
| N(4)  | 19(1)    | 20(1)    | 23(1)    | 1(1)     | 9(1)     | 2(1)     |
| C(1)  | 23(1)    | 23(1)    | 27(1)    | 1(1)     | 12(1)    | 8(1)     |
| C(2)  | 30(1)    | 23(1)    | 32(1)    | -5(1)    | 18(1)    | 2(1)     |
| C(3)  | 28(1)    | 45(1)    | 24(1)    | -10(1)   | 10(1)    | 6(1)     |
| C(4)  | 36(1)    | 50(2)    | 25(1)    | 9(1)     | 18(1)    | 19(1)    |
| C(5)  | 34(1)    | 29(1)    | 46(2)    | 11(1)    | 30(1)    | 11(1)    |
| C(6)  | 61(2)    | 36(2)    | 100(3)   | 26(2)    | 60(2)    | 12(1)    |
| C(7)  | 19(1)    | 26(1)    | 38(1)    | -3(1)    | 15(1)    | 3(1)     |
| C(8)  | 40(2)    | 24(1)    | 65(2)    | -10(1)   | 31(2)    | -5(1)    |
| C(9)  | 75(3)    | 31(2)    | 97(3)    | -25(2)   | 49(2)    | -10(2)   |
| C(10) | 82(3)    | 28(1)    | 75(2)    | 14(2)    | 51(2)    | 5(2)     |
| C(11) | 20(1)    | 20(1)    | 25(1)    | -2(1)    | 11(1)    | -1(1)    |
| C(12) | 19(1)    | 27(1)    | 35(1)    | -4(1)    | 12(1)    | 1(1)     |
| C(13) | 23(1)    | 26(1)    | 30(1)    | 0(1)     | 5(1)     | 5(1)     |
| C(14) | 28(1)    | 22(1)    | 23(1)    | 2(1)     | 9(1)     | 1(1)     |
| C(15) | 22(1)    | 19(1)    | 26(1)    | -2(1)    | 12(1)    | -1(1)    |
| C(16) | 23(1)    | 25(1)    | 28(1)    | 2(1)     | 13(1)    | -1(1)    |
| C(17) | 38(2)    | 28(1)    | 41(1)    | -1(1)    | 26(1)    | -1(1)    |
| C(18) | 49(2)    | 39(1)    | 44(2)    | -4(1)    | 33(1)    | -1(1)    |
| C(19) | 37(2)    | 43(2)    | 40(1)    | 11(1)    | 24(1)    | 0(1)     |
| C(20) | 26(1)    | 28(1)    | 37(1)    | 7(1)     | 13(1)    | -2(1)    |
| C(21) | 22(1)    | 25(1)    | 27(1)    | 3(1)     | 9(1)     | 0(1)     |
| C(22) | 44(2)    | 23(1)    | 48(2)    | -1(1)    | 14(1)    | -2(1)    |

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for 5.

|        | x    | y     | z    | U(eq) |
|--------|------|-------|------|-------|
| H(1)   | 5344 | 7418  | 5537 | 28    |
| H(3)   | 7299 | 7324  | 8340 | 39    |
| H(4)   | 6868 | 5051  | 8669 | 42    |
| H(6A)  | 6015 | 2866  | 8001 | 86    |
| H(6B)  | 5279 | 2912  | 6905 | 86    |
| H(6C)  | 5159 | 3543  | 7892 | 86    |
| H(7)   | 4903 | 5200  | 5916 | 32    |
| H(8)   | 7335 | 8909  | 6872 | 48    |
| H(9A)  | 6808 | 11098 | 7187 | 94    |
| H(9B)  | 6750 | 9955  | 7995 | 94    |
| H(9C)  | 5952 | 10372 | 7022 | 94    |
| H(10A) | 6487 | 8583  | 5091 | 83    |
| H(10B) | 6690 | 10218 | 5377 | 83    |
| H(10C) | 5817 | 9593  | 5243 | 83    |
| H(12)  | 9625 | 4183  | 7081 | 32    |
| H(13)  | 9443 | 2604  | 8442 | 33    |
| H(14)  | 8003 | 2994  | 8371 | 29    |
| H(17)  | 8604 | 4386  | 4643 | 39    |
| H(18)  | 9166 | 5208  | 3463 | 47    |
| H(19)  | 9447 | 7643  | 3408 | 44    |
| H(20)  | 9186 | 9263  | 4511 | 36    |
| H(22A) | 9295 | 10329 | 6134 | 59    |
| H(22B) | 8509 | 10669 | 6391 | 59    |
| H(22C) | 8425 | 10539 | 5223 | 59    |





**Table 3.** Hydrogen bonding distances and angles for **2-5** (Å and °).

| D-H...A       | d(D-H) | d(H...A) | d(D...A)   | <(DHA) |
|---------------|--------|----------|------------|--------|
| <b>2</b>      |        |          |            |        |
| C1-H1B...Cl1  | 0.9800 | 2.8100   | 3.4603(19) | 125.00 |
| C3-H3...O1#1  | 0.9500 | 2.4900   | 3.1721(19) | 128.00 |
| C4-H4...Cl1#1 | 0.9500 | 2.8100   | 3.7475(16) | 170.00 |
| C8-H...O2     | 1.0000 | 2.5100   | 3.366(2)   | 143.00 |
| <b>3</b>      |        |          |            |        |
| C13-H13...Cl1 | 0.9300 | 2.6900   | 3.545(8)   | 153.00 |
| C33-H33...Cl1 | 0.9300 | 2.6900   | 3.415(8)   | 135.00 |
| C39-H39...O2  | 0.9300 | 2.5300   | 2.988(9)   | 111.00 |
| <b>4</b>      |        |          |            |        |
| C20-H20...O1  | 0.9800 | 2.5400   | 3.425(7)   | 150.00 |
| <b>5</b>      |        |          |            |        |
| C6-H6A...N3#2 | 0.9600 | 2.5900   | 3.488(5)   | 155.00 |
| C7-H7...N1#3  | 0.9300 | 2.5400   | 3.226(3)   | 131.00 |
| C10-H10A...O1 | 0.9600 | 2.5500   | 3.270(4)   | 132.00 |

Symmetry transformations used to generate equivalent atoms:

#1 1-x,1-y,-z; #2 x,1/2-y,1/2+z; #3 1-x,1-y,1-z