

EXPERIMENTAL DETAILS

A. Crystal Data

| | |
|--|---|
| Empirical Formula | $C_{36}H_{30}N_{24}Ru_2$ |
| Formula Weight | 1000.93 |
| Crystal Color, Habit | deep, plate |
| Crystal Dimensions | 0.12 X 0.25 X 0.26 mm |
| Crystal System | monoclinic |
| Lattice Type | Primitive |
| No. of Reflections Used for Unit Cell Determination (2θ range) | 25 (58.9 - 59.9°) |
| Omega Scan Peak Width at Half-height | 0.36° |
| Lattice Parameters | $a = 12.2426(8) \text{ \AA}$ $b = 12.643(1) \text{ \AA}$ $c = 13.2066(6) \text{ \AA}$ $\beta = 92.738(4)^\circ$ $V = 2041.8(2) \text{ \AA}^3$ |
| Space Group | $P2_1$ (#4) |
| Z value | 2 |
| D_{calc} | 1.628 g/cm ³ |
| F_{000} | 1004.00 |
| $\mu(CuK\alpha)$ | 65.12 cm ⁻¹ |

B. Intensity Measurements

| | |
|----------------|---|
| Diffractometer | Rigaku AFC7R (rotating anode) |
| Radiation | $CuK\alpha$ ($\lambda = 1.54178 \text{ \AA}$) graphite monochromated |
| Attenuator | Ni foil (factor = 9.14) |

| | |
|------------------------------|---|
| Temperature | 23.0 °C |
| Collimator Size | 1.0 mm |
| Take-off Angle | 6.0° |
| Detector Aperture | 9.0 mm horizontal 13.0 mm vertical |
| Crystal to Detector Distance | 235 mm |
| Scan Type | ω - 2θ |
| Scan Rate | 16.0°/min (in ω) (up to 5 scans) |
| Scan Width | $(1.68 + 0.30 \tan \theta)^\circ$ |
| $2\theta_{max}$ | 120.2° |
| No. of Reflections Measured | Total: 3360 Unique: 3194 ($R_{int} = 0.041$) |
| Corrections | Lorentz-polarization Absorption (trans. factors: 0.5343 - 0.9994) Decay (0.96% increase) Secondary Extinction (coefficient: 6.37500e-07) |

C. Structure Solution and Refinement

| | |
|--|--|
| Structure Solution | Direct Methods (SHELXS-86) |
| Refinement | Full-matrix least-squares |
| Function Minimized | $\Sigma w(F_o - F_c)^2$ |
| Least Squares Weights | $w = \frac{1}{\sigma^2(F_o)} = [\sigma_c^2(F_o) + \frac{v^2}{4} F_o^2]^{-1}$ |
| p-factor | 0.0030 |
| Anomalous Dispersion | All non-hydrogen atoms |
| No. of Observations ($I > 3.00\sigma(I)$, $2\theta < 120.20^\circ$) | 2776 |
| No. Variables | 560 |
| Reflection/Parameter Ratio | 4.96 |
| Residuals: R; Rw | 0.042 ; 0.067 |

| | |
|---------------------------------|----------------------------|
| Residuals: R1 | 0.042 |
| No. of Reflections to calc R1 | 2636 |
| Goodness of Fit Indicator | 1.75 |
| Max Shift/Error in Final Cycle | 0.684 |
| Maximum peak in Final Diff. Map | $0.72 e^{-}/\text{\AA}^3$ |
| Minimum peak in Final Diff. Map | $-1.46 e^{-}/\text{\AA}^3$ |

Table 1. Atomic coordinates and B_{iso}/B_{eq}

| atom | x | y | z | B_{eq} |
|-------|-------------|-------------|------------|----------|
| Ru(1) | -0.39091(6) | 0.19991(10) | 0.90562(6) | 3.06(2) |
| Ru(2) | 0.10811(7) | 0.00990(10) | 0.40632(6) | 3.46(2) |
| N(1) | -0.5527(7) | 0.1511(8) | 0.8665(8) | 4.3(2) |
| N(2) | -0.7115(8) | 0.1991(8) | 0.8005(8) | 4.5(2) |
| N(3) | -0.4597(8) | 0.3398(6) | 0.8465(5) | 2.8(1) |
| N(4) | -0.5966(8) | 0.4222(7) | 0.7633(8) | 4.1(2) |
| N(5) | -0.3324(7) | 0.0582(6) | 0.9471(6) | 2.8(1) |
| N(6) | -0.2493(9) | -0.0921(8) | 0.8992(8) | 4.4(2) |
| N(7) | -0.3431(9) | 0.1447(7) | 0.7691(7) | 4.2(2) |
| N(8) | -0.3088(9) | -0.0021(9) | 0.6795(8) | 4.5(2) |
| N(9) | -0.2446(7) | 0.2592(7) | 0.9704(5) | 2.9(1) |
| N(10) | -0.1594(9) | 0.3230(9) | 1.1130(7) | 4.7(2) |
| N(11) | -0.4329(7) | 0.2388(7) | 1.0396(6) | 3.5(1) |
| N(12) | -0.3953(9) | 0.3092(8) | 1.1969(8) | 5.1(2) |
| N(13) | 0.1816(8) | 0.1593(7) | 0.4453(8) | 3.9(2) |
| N(14) | 0.2627(9) | 0.3047(7) | 0.4051(7) | 3.7(2) |
| N(15) | 0.1553(6) | 0.0730(7) | 0.2660(7) | 3.3(1) |
| N(16) | 0.2015(8) | 0.2128(7) | 0.1795(6) | 3.4(2) |
| N(17) | -0.0402(7) | 0.0574(6) | 0.3567(5) | 2.6(1) |
| N(18) | -0.2115(8) | 0.0210(8) | 0.3008(6) | 4.0(2) |
| N(19) | 0.0485(7) | -0.1233(8) | 0.3458(8) | 4.5(2) |
| N(20) | -0.0960(9) | -0.2067(8) | 0.2646(7) | 4.4(2) |
| N(21) | 0.2518(7) | -0.0523(7) | 0.4715(8) | 3.8(2) |
| N(22) | 0.3428(7) | -0.1072(7) | 0.6077(8) | 3.7(2) |

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

| atom | x | y | z | B_{eq} |
|-------|-------------|------------|------------|----------|
| N(23) | 0.0547(6) | -0.0288(7) | 0.5540(5) | 3.3(1) |
| N(24) | 0.1035(7) | -0.0905(7) | 0.7043(6) | 3.1(2) |
| C(1) | -0.612(1) | 0.0707(9) | 0.8584(10) | 5.4(3) |
| C(2) | -0.709(1) | 0.090(1) | 0.828(1) | 6.1(3) |
| C(3) | -0.421(1) | 0.4447(9) | 0.826(1) | 4.6(3) |
| C(4) | -0.513(1) | 0.498(1) | 0.782(1) | 5.7(3) |
| C(5) | -0.6072(9) | 0.2273(9) | 0.8147(8) | 3.4(2) |
| C(6) | -0.555(1) | 0.3274(9) | 0.7988(9) | 3.4(2) |
| C(7) | -0.296(1) | -0.002(1) | 1.0315(9) | 5.0(3) |
| C(8) | -0.251(1) | -0.084(1) | 1.009(1) | 5.2(3) |
| C(9) | -0.366(1) | 0.167(1) | 0.6655(9) | 4.7(3) |
| C(10) | -0.334(1) | 0.078(1) | 0.613(1) | 4.5(3) |
| C(11) | -0.2938(9) | -0.0049(8) | 0.8614(7) | 3.2(2) |
| C(12) | -0.3096(8) | 0.0433(8) | 0.7683(9) | 3.1(2) |
| C(13) | -0.1420(10) | 0.2708(9) | 0.9498(9) | 3.8(2) |
| C(14) | -0.0838(9) | 0.306(1) | 1.0378(9) | 5.1(3) |
| C(15) | -0.5336(8) | 0.2388(8) | 1.1089(8) | 3.5(2) |
| C(16) | -0.501(1) | 0.285(1) | 1.1950(9) | 4.2(2) |
| C(17) | -0.2528(8) | 0.2922(7) | 1.0674(7) | 2.6(2) |
| C(18) | -0.3678(9) | 0.2786(8) | 1.112(1) | 4.4(2) |
| C(19) | 0.2078(10) | 0.2039(10) | 0.5353(9) | 4.1(2) |
| C(20) | 0.261(1) | 0.3043(9) | 0.5033(9) | 4.5(2) |
| C(21) | 0.1424(10) | 0.0477(8) | 0.1708(9) | 3.8(2) |
| C(22) | 0.166(1) | 0.131(1) | 0.1146(8) | 5.1(3) |

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

| atom | x | y | z | B_{eq} |
|-------|-------------|------------|------------|----------|
| C(23) | 0.2061(9) | 0.2129(8) | 0.3788(8) | 3.6(2) |
| C(24) | 0.189(1) | 0.1755(9) | 0.2715(8) | 3.9(2) |
| C(25) | -0.1100(9) | 0.1515(8) | 0.3771(9) | 3.5(2) |
| C(26) | -0.2147(9) | 0.1199(10) | 0.330(1) | 4.1(2) |
| C(27) | 0.0729(9) | -0.2245(9) | 0.3311(10) | 3.6(2) |
| C(28) | -0.0089(10) | -0.2710(8) | 0.2764(7) | 3.2(2) |
| C(29) | -0.113(1) | -0.0194(9) | 0.3242(7) | 3.1(2) |
| C(30) | -0.0633(9) | -0.1211(9) | 0.3119(9) | 3.3(2) |
| C(31) | 0.3648(10) | -0.069(1) | 0.452(1) | 4.5(2) |
| C(32) | 0.4149(10) | -0.106(1) | 0.5375(9) | 4.8(2) |
| C(33) | -0.0277(7) | -0.0337(9) | 0.5883(8) | 3.9(2) |
| C(34) | -0.0088(9) | -0.066(1) | 0.6913(10) | 4.1(2) |
| C(35) | 0.2421(9) | -0.077(1) | 0.571(1) | 4.6(2) |
| C(36) | 0.1488(8) | -0.0675(8) | 0.6086(5) | 2.6(1) |
| H(1) | -0.7721 | 0.2350 | 0.7663 | 4.9 |
| H(2) | -0.5854 | -0.0005 | 0.8721 | 5.6 |
| H(3) | -0.7775 | 0.0397 | 0.8412 | 7.1 |
| H(4) | -0.3369 | 0.4721 | 0.8386 | 6.9 |
| H(5) | -0.5115 | 0.5756 | 0.7577 | 7.2 |
| H(6) | -0.2251 | -0.1534 | 0.8629 | 4.1 |
| H(7) | -0.3128 | 0.0170 | 1.1028 | 4.3 |
| H(8) | -0.2161 | -0.1327 | 1.0525 | 4.1 |
| H(9) | -0.3867 | 0.2323 | 0.6387 | 3.7 |
| H(10) | -0.3233 | 0.0738 | 0.5400 | 4.5 |

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

| atom | x | y | z | B_{eq} |
|-------|---------|---------|--------|----------|
| H(11) | -0.1452 | 0.3505 | 1.1836 | 5.5 |
| H(12) | -0.1136 | 0.2535 | 0.8816 | 4.1 |
| H(13) | -0.0079 | 0.3304 | 1.0420 | 4.6 |
| H(14) | -0.6099 | 0.2143 | 1.0888 | 4.2 |
| H(15) | -0.5411 | 0.2979 | 1.2517 | 4.7 |
| H(16) | 0.2974 | 0.3526 | 0.3569 | 4.3 |
| H(17) | 0.1989 | 0.1747 | 0.6047 | 6.0 |
| H(18) | 0.2962 | 0.3653 | 0.5489 | 6.5 |
| H(19) | 0.1125 | -0.0242 | 0.1367 | 5.8 |
| H(20) | 0.1457 | 0.1411 | 0.0436 | 5.3 |
| H(21) | -0.2709 | -0.0233 | 0.2738 | 4.6 |
| H(22) | -0.0903 | 0.2185 | 0.4119 | 4.0 |
| H(23) | -0.2761 | 0.1644 | 0.3127 | 3.8 |
| H(24) | 0.1371 | -0.2607 | 0.3552 | 2.8 |
| H(25) | -0.0127 | -0.3416 | 0.2525 | 3.7 |
| H(26) | 0.3557 | -0.1318 | 0.6755 | 3.8 |
| H(27) | 0.4050 | -0.0630 | 0.3924 | 5.4 |
| H(28) | 0.4983 | -0.1116 | 0.5515 | 6.9 |
| H(29) | -0.0960 | -0.0140 | 0.5524 | 4.3 |
| H(30) | -0.0685 | -0.0764 | 0.7445 | 4.3 |

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos \gamma + 2U_{13}aa^*cc^* \cos \beta + 2U_{23}bb^*cc^* \cos \alpha)$$

Table 2. Anisotropic Displacement Parameters

| atom | U ₁₁ | U ₂₂ | U ₃₃ | U ₁₂ | U ₁₃ | U ₂₃ |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Ru(1) | 0.0363(4) | 0.0316(4) | 0.0476(5) | 0.0040(4) | -0.0076(4) | -0.0044(3) |
| Ru(2) | 0.0505(6) | 0.0362(5) | 0.0426(5) | -0.0079(4) | -0.0189(5) | 0.0095(3) |
| N(1) | 0.034(3) | 0.049(4) | 0.079(6) | 0.003(3) | -0.010(4) | 0.014(4) |
| N(2) | 0.047(4) | 0.043(4) | 0.081(7) | -0.020(4) | -0.016(5) | 0.019(5) |
| N(3) | 0.059(5) | 0.028(3) | 0.018(3) | 0.006(3) | -0.001(3) | -0.015(3) |
| N(4) | 0.046(5) | 0.035(4) | 0.073(6) | 0.024(3) | -0.020(5) | -0.019(4) |
| N(5) | 0.044(4) | 0.039(3) | 0.026(3) | 0.016(3) | 0.017(3) | -0.009(3) |
| N(6) | 0.067(6) | 0.041(5) | 0.059(4) | 0.021(4) | -0.012(5) | -0.004(4) |
| N(7) | 0.094(7) | 0.026(4) | 0.035(3) | 0.017(4) | -0.025(4) | 0.005(3) |
| N(8) | 0.052(6) | 0.051(6) | 0.069(5) | 0.003(5) | 0.006(5) | -0.008(4) |
| N(9) | 0.049(3) | 0.046(5) | 0.014(3) | -0.002(3) | -0.017(3) | 0.004(3) |
| N(10) | 0.061(5) | 0.087(8) | 0.028(4) | -0.008(6) | -0.013(4) | -0.013(5) |
| N(11) | 0.037(3) | 0.032(4) | 0.068(3) | 0.005(3) | 0.037(3) | 0.000(3) |
| N(12) | 0.066(5) | 0.052(6) | 0.071(5) | -0.010(5) | -0.039(5) | 0.013(4) |
| N(13) | 0.056(6) | 0.032(3) | 0.058(4) | 0.004(3) | -0.022(5) | -0.001(3) |
| N(14) | 0.060(6) | 0.035(4) | 0.043(3) | -0.001(4) | -0.016(4) | 0.004(4) |
| N(15) | 0.018(3) | 0.047(4) | 0.061(3) | 0.007(3) | -0.004(3) | 0.019(3) |
| N(16) | 0.063(5) | 0.033(4) | 0.032(4) | -0.008(4) | -0.013(4) | 0.009(3) |
| N(17) | 0.058(3) | 0.020(3) | 0.018(3) | 0.003(3) | -0.013(3) | 0.011(3) |
| N(18) | 0.064(5) | 0.046(4) | 0.037(4) | -0.014(4) | -0.026(4) | 0.020(4) |
| N(19) | 0.025(4) | 0.044(4) | 0.098(7) | -0.003(3) | -0.022(4) | -0.014(4) |
| N(20) | 0.057(6) | 0.057(5) | 0.054(6) | 0.019(4) | -0.003(5) | -0.027(4) |
| N(21) | 0.035(3) | 0.028(4) | 0.081(5) | -0.018(3) | 0.001(3) | 0.014(4) |
| N(22) | 0.031(4) | 0.039(5) | 0.069(6) | -0.002(4) | -0.016(3) | 0.011(4) |

Table 2. Anisotropic Displacement Parameters (continued)

| atom | U_{11} | U_{22} | U_{33} | U_{12} | U_{13} | U_{23} |
|-------|----------|----------|----------|-----------|-----------|-----------|
| N(23) | 0.033(3) | 0.047(5) | 0.041(2) | -0.015(3) | -0.038(2) | 0.020(3) |
| N(24) | 0.031(3) | 0.048(5) | 0.039(4) | -0.021(3) | 0.015(3) | 0.020(4) |
| C(1) | 0.116(8) | 0.025(5) | 0.060(6) | -0.012(4) | -0.049(6) | 0.008(4) |
| C(2) | 0.110(8) | 0.036(5) | 0.08(1) | -0.022(7) | -0.038(9) | -0.001(6) |
| C(3) | 0.083(8) | 0.029(4) | 0.062(7) | -0.005(5) | -0.010(7) | 0.001(5) |
| C(4) | 0.062(7) | 0.035(6) | 0.12(1) | -0.001(4) | 0.004(7) | -0.012(6) |
| C(5) | 0.044(4) | 0.036(5) | 0.048(6) | -0.006(4) | -0.014(5) | -0.010(4) |
| C(6) | 0.051(5) | 0.028(4) | 0.048(5) | 0.010(3) | -0.003(4) | -0.008(4) |
| C(7) | 0.089(9) | 0.060(7) | 0.039(5) | 0.016(6) | -0.032(6) | 0.002(4) |
| C(8) | 0.082(9) | 0.059(7) | 0.057(4) | 0.014(6) | 0.003(6) | 0.031(5) |
| C(9) | 0.082(9) | 0.066(7) | 0.030(4) | -0.002(7) | -0.015(6) | 0.003(5) |
| C(10) | 0.053(7) | 0.058(6) | 0.061(7) | -0.012(5) | -0.010(6) | -0.006(4) |
| C(11) | 0.051(5) | 0.034(4) | 0.038(4) | 0.019(4) | -0.006(4) | -0.030(3) |
| C(12) | 0.030(5) | 0.027(4) | 0.061(4) | 0.000(4) | -0.006(5) | 0.009(3) |
| C(13) | 0.046(4) | 0.045(6) | 0.051(6) | 0.004(5) | -0.016(4) | -0.007(5) |
| C(14) | 0.040(6) | 0.092(8) | 0.060(6) | 0.019(6) | -0.016(4) | -0.051(6) |
| C(15) | 0.040(5) | 0.040(5) | 0.055(5) | 0.006(4) | 0.033(4) | -0.008(4) |
| C(16) | 0.062(5) | 0.045(7) | 0.052(5) | 0.016(5) | 0.022(5) | -0.009(5) |
| C(17) | 0.048(4) | 0.024(5) | 0.029(3) | 0.018(4) | 0.003(3) | -0.003(4) |
| C(18) | 0.032(4) | 0.027(5) | 0.108(7) | 0.011(4) | 0.008(4) | -0.014(5) |
| C(19) | 0.057(6) | 0.042(5) | 0.058(5) | -0.001(5) | 0.000(5) | -0.011(4) |
| C(20) | 0.087(9) | 0.040(6) | 0.042(3) | -0.019(5) | -0.033(6) | 0.001(5) |
| C(21) | 0.048(6) | 0.027(5) | 0.069(5) | -0.009(5) | -0.014(6) | -0.004(4) |
| C(22) | 0.11(1) | 0.056(6) | 0.024(5) | -0.035(7) | -0.018(6) | -0.002(4) |

Table 2. Anisotropic Displacement Parameters (continued)

| atom | U ₁₁ | U ₂₂ | U ₃₃ | U ₁₂ | U ₁₃ | U ₂₃ |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| C(23) | 0.050(6) | 0.040(5) | 0.043(4) | 0.012(4) | -0.025(4) | -0.013(3) |
| C(24) | 0.061(7) | 0.053(5) | 0.033(3) | -0.020(5) | -0.013(6) | 0.015(4) |
| C(25) | 0.035(4) | 0.032(4) | 0.064(6) | -0.001(3) | -0.008(4) | -0.003(4) |
| C(26) | 0.030(4) | 0.047(5) | 0.078(8) | -0.005(5) | -0.011(5) | 0.005(6) |
| C(27) | 0.027(4) | 0.044(4) | 0.064(7) | -0.001(4) | 0.006(4) | 0.008(5) |
| C(28) | 0.057(5) | 0.024(5) | 0.040(5) | -0.007(3) | 0.001(4) | -0.011(4) |
| C(29) | 0.061(5) | 0.037(4) | 0.018(4) | -0.014(3) | -0.010(4) | 0.006(4) |
| C(30) | 0.030(4) | 0.047(4) | 0.046(5) | 0.001(4) | -0.015(4) | 0.017(4) |
| C(31) | 0.039(4) | 0.067(8) | 0.065(7) | -0.004(5) | 0.009(5) | -0.006(6) |
| C(32) | 0.043(6) | 0.074(7) | 0.062(5) | 0.017(5) | -0.005(4) | -0.034(5) |
| C(33) | 0.025(3) | 0.062(6) | 0.058(5) | 0.000(4) | -0.038(3) | -0.018(4) |
| C(34) | 0.040(4) | 0.049(7) | 0.064(5) | 0.000(5) | -0.024(5) | 0.001(5) |
| C(35) | 0.036(4) | 0.059(8) | 0.076(6) | 0.011(5) | -0.026(4) | 0.011(6) |
| C(36) | 0.051(4) | 0.040(5) | 0.004(3) | 0.004(4) | -0.029(2) | 0.001(3) |

The general temperature factor expression:

$$\exp(-2\pi^2(a^*U_{11}h^2 + b^*U_{22}k^2 + c^*U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths(\AA)

| atom | atom | distance | atom | atom | distance |
|-------|-------|----------|-------|-------|-----------|
| Ru(1) | N(1) | 2.115(9) | Ru(1) | N(3) | 2.093(8) |
| Ru(1) | N(5) | 1.996(8) | Ru(1) | N(7) | 2.045(9) |
| Ru(1) | N(9) | 2.087(9) | Ru(1) | N(11) | 1.929(9) |
| Ru(2) | N(13) | 2.144(9) | Ru(2) | N(15) | 2.122(10) |
| Ru(2) | N(17) | 1.993(8) | Ru(2) | N(19) | 1.987(10) |
| Ru(2) | N(21) | 2.076(9) | Ru(2) | N(23) | 2.144(7) |
| N(1) | C(1) | 1.25(2) | N(1) | C(5) | 1.34(1) |
| N(2) | C(2) | 1.42(2) | N(2) | C(5) | 1.33(1) |
| N(2) | H(1) | 0.96 | N(3) | C(3) | 1.44(1) |
| N(3) | C(6) | 1.31(1) | N(4) | C(4) | 1.41(2) |
| N(4) | C(6) | 1.38(1) | N(5) | C(7) | 1.40(1) |
| N(5) | C(11) | 1.48(1) | N(6) | C(8) | 1.45(2) |
| N(6) | C(11) | 1.32(1) | N(6) | H(6) | 0.96 |
| N(7) | C(9) | 1.41(1) | N(7) | C(12) | 1.35(1) |
| N(8) | C(10) | 1.36(2) | N(8) | C(12) | 1.31(2) |
| N(9) | C(13) | 1.31(2) | N(9) | C(17) | 1.36(1) |
| N(10) | C(14) | 1.41(2) | N(10) | C(17) | 1.33(1) |
| N(10) | H(11) | 1.00 | N(11) | C(15) | 1.57(1) |
| N(11) | C(18) | 1.32(1) | N(12) | C(16) | 1.33(2) |
| N(12) | C(18) | 1.24(2) | N(13) | C(19) | 1.34(2) |
| N(13) | C(23) | 1.16(1) | N(14) | C(20) | 1.30(1) |
| N(14) | C(23) | 1.39(1) | N(14) | H(16) | 0.99 |
| N(15) | C(21) | 1.30(2) | N(15) | C(24) | 1.36(2) |
| N(16) | C(22) | 1.40(2) | N(16) | C(24) | 1.32(1) |

Table 3. Bond Lengths(\AA) (continued)

| atom | atom | distance | atom | atom | distance |
|-------|-------|----------|-------|-------|----------|
| N(17) | C(25) | 1.50(1) | N(17) | C(29) | 1.37(1) |
| N(18) | C(26) | 1.31(2) | N(18) | C(29) | 1.34(2) |
| N(18) | H(21) | 0.97 | N(19) | C(27) | 1.33(2) |
| N(19) | C(30) | 1.42(1) | N(20) | C(28) | 1.34(2) |
| N(20) | C(30) | 1.30(2) | N(21) | C(31) | 1.44(2) |
| N(21) | C(35) | 1.37(2) | N(22) | C(32) | 1.31(2) |
| N(22) | C(35) | 1.36(1) | N(22) | H(26) | 0.95 |
| N(23) | C(33) | 1.13(1) | N(23) | C(36) | 1.42(1) |
| N(24) | C(34) | 1.41(1) | N(24) | C(36) | 1.43(1) |
| C(1) | C(2) | 1.26(2) | C(1) | H(2) | 0.97 |
| C(2) | H(3) | 1.08 | C(3) | C(4) | 1.41(2) |
| C(3) | H(4) | 1.10 | C(4) | H(5) | 1.04 |
| C(5) | C(6) | 1.44(2) | C(7) | C(8) | 1.22(2) |
| C(7) | H(7) | 1.00 | C(8) | H(8) | 0.93 |
| C(9) | C(10) | 1.38(2) | C(9) | H(9) | 0.93 |
| C(10) | H(10) | 0.99 | C(11) | C(12) | 1.38(1) |
| C(13) | C(14) | 1.41(2) | C(13) | H(12) | 1.00 |
| C(14) | H(13) | 0.98 | C(15) | C(16) | 1.33(2) |
| C(15) | H(14) | 1.01 | C(16) | H(15) | 0.93 |
| C(17) | C(18) | 1.56(2) | C(19) | C(20) | 1.50(2) |
| C(19) | H(17) | 1.00 | C(20) | H(18) | 1.06 |
| C(21) | C(22) | 1.33(2) | C(21) | H(19) | 1.07 |
| C(22) | H(20) | 0.97 | C(23) | C(24) | 1.50(2) |
| C(25) | C(26) | 1.46(2) | C(25) | H(22) | 0.99 |

Table 3. Bond Lengths(\AA) (continued)

| atom | atom | distance | atom | atom | distance |
|-------|-------|----------|-------|-------|----------|
| C(26) | H(23) | 0.96 | C(27) | C(28) | 1.34(2) |
| C(27) | H(24) | 0.95 | C(28) | H(25) | 0.95 |
| C(29) | C(30) | 1.43(2) | C(31) | C(32) | 1.34(2) |
| C(31) | H(27) | 0.95 | C(32) | H(28) | 1.03 |
| C(33) | C(34) | 1.43(2) | C(33) | H(29) | 0.97 |
| C(34) | H(30) | 1.05 | C(35) | C(36) | 1.27(1) |

Table 4. Bond Angles(°)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|----------|-------|-------|-------|-----------|
| N(1) | Ru(1) | N(3) | 78.5(4) | N(1) | Ru(1) | N(5) | 97.2(4) |
| N(1) | Ru(1) | N(7) | 89.4(4) | N(1) | Ru(1) | N(9) | 168.6(4) |
| N(1) | Ru(1) | N(11) | 90.6(4) | N(3) | Ru(1) | N(5) | 173.2(3) |
| N(3) | Ru(1) | N(7) | 95.0(3) | N(3) | Ru(1) | N(9) | 99.9(3) |
| N(3) | Ru(1) | N(11) | 90.4(3) | N(5) | Ru(1) | N(7) | 79.7(3) |
| N(5) | Ru(1) | N(9) | 85.4(3) | N(5) | Ru(1) | N(11) | 94.9(3) |
| N(7) | Ru(1) | N(9) | 102.0(4) | N(7) | Ru(1) | N(11) | 174.5(4) |
| N(9) | Ru(1) | N(11) | 78.1(3) | N(13) | Ru(2) | N(15) | 75.5(4) |
| N(13) | Ru(2) | N(17) | 100.3(3) | N(13) | Ru(2) | N(19) | 169.9(4) |
| N(13) | Ru(2) | N(21) | 84.0(4) | N(13) | Ru(2) | N(23) | 97.2(4) |
| N(15) | Ru(2) | N(17) | 83.2(3) | N(15) | Ru(2) | N(19) | 94.4(4) |
| N(15) | Ru(2) | N(21) | 104.1(4) | N(15) | Ru(2) | N(23) | 171.0(3) |
| N(17) | Ru(2) | N(19) | 79.2(3) | N(17) | Ru(2) | N(21) | 172.3(3) |
| N(17) | Ru(2) | N(23) | 93.1(3) | N(19) | Ru(2) | N(21) | 97.7(4) |
| N(19) | Ru(2) | N(23) | 92.9(4) | N(21) | Ru(2) | N(23) | 79.9(4) |
| Ru(1) | N(1) | C(1) | 142.1(9) | Ru(1) | N(1) | C(5) | 110.6(8) |
| C(1) | N(1) | C(5) | 105(1) | C(2) | N(2) | C(5) | 102(1) |
| C(2) | N(2) | H(1) | 125.7 | C(5) | N(2) | H(1) | 130.7 |
| Ru(1) | N(3) | C(3) | 136.1(8) | Ru(1) | N(3) | C(6) | 114.4(7) |
| C(3) | N(3) | C(6) | 108.1(9) | C(4) | N(4) | C(6) | 106.1(10) |
| Ru(1) | N(5) | C(7) | 143.2(7) | Ru(1) | N(5) | C(11) | 113.4(6) |
| C(7) | N(5) | C(11) | 102.3(8) | C(8) | N(6) | C(11) | 107.0(10) |
| C(8) | N(6) | H(6) | 124.9 | C(11) | N(6) | H(6) | 127.9 |
| Ru(1) | N(7) | C(9) | 137.1(9) | Ru(1) | N(7) | C(12) | 115.6(7) |

Table 4. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|-----------|-------|-------|-------|----------|
| C(9) | N(7) | C(12) | 103.3(9) | C(10) | N(8) | C(12) | 103(1) |
| Ru(1) | N(9) | C(13) | 140.4(7) | Ru(1) | N(9) | C(17) | 113.4(7) |
| C(13) | N(9) | C(17) | 106.1(9) | C(14) | N(10) | C(17) | 102.5(9) |
| C(14) | N(10) | H(11) | 128.2 | C(17) | N(10) | H(11) | 129.2 |
| Ru(1) | N(11) | C(15) | 141.8(6) | Ru(1) | N(11) | C(18) | 126.0(8) |
| C(15) | N(11) | C(18) | 92.2(8) | C(16) | N(12) | C(18) | 102(1) |
| Ru(2) | N(13) | C(19) | 131.5(8) | Ru(2) | N(13) | C(23) | 117.0(8) |
| C(19) | N(13) | C(23) | 111(1) | C(20) | N(14) | C(23) | 102.5(9) |
| C(20) | N(14) | H(16) | 132.2 | C(23) | N(14) | H(16) | 125.2 |
| Ru(2) | N(15) | C(21) | 136.6(8) | Ru(2) | N(15) | C(24) | 114.0(7) |
| C(21) | N(15) | C(24) | 107.9(9) | C(22) | N(16) | C(24) | 104.7(9) |
| Ru(2) | N(17) | C(25) | 134.4(6) | Ru(2) | N(17) | C(29) | 117.0(7) |
| C(25) | N(17) | C(29) | 104.7(8) | C(26) | N(18) | C(29) | 109.7(9) |
| C(26) | N(18) | H(21) | 128.7 | C(29) | N(18) | H(21) | 121.2 |
| Ru(2) | N(19) | C(27) | 142.5(8) | Ru(2) | N(19) | C(30) | 116.1(7) |
| C(27) | N(19) | C(30) | 101.1(9) | C(28) | N(20) | C(30) | 102.8(9) |
| Ru(2) | N(21) | C(31) | 141.8(9) | Ru(2) | N(21) | C(35) | 112.0(7) |
| C(31) | N(21) | C(35) | 105.7(10) | C(32) | N(22) | C(35) | 112(1) |
| C(32) | N(22) | H(26) | 125.6 | C(35) | N(22) | H(26) | 122.1 |
| Ru(2) | N(23) | C(33) | 134.1(7) | Ru(2) | N(23) | C(36) | 105.4(5) |
| C(33) | N(23) | C(36) | 119.9(8) | C(34) | N(24) | C(36) | 105.4(8) |
| N(1) | C(1) | C(2) | 113(1) | N(1) | C(1) | H(2) | 123.8 |
| C(2) | C(1) | H(2) | 122.7 | N(2) | C(2) | C(1) | 106(1) |
| N(2) | C(2) | H(3) | 127.2 | C(1) | C(2) | H(3) | 124.4 |

Table 4. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|-----------|-------|-------|-------|----------|
| N(3) | C(3) | C(4) | 104(1) | N(3) | C(3) | H(4) | 125.3 |
| C(4) | C(3) | H(4) | 129.7 | N(4) | C(4) | C(3) | 107(1) |
| N(4) | C(4) | H(5) | 127.7 | C(3) | C(4) | H(5) | 123.8 |
| N(1) | C(5) | N(2) | 109.3(10) | N(1) | C(5) | C(6) | 119(1) |
| N(2) | C(5) | C(6) | 130(1) | N(3) | C(6) | N(4) | 111.5(9) |
| N(3) | C(6) | C(5) | 115.3(10) | N(4) | C(6) | C(5) | 131(1) |
| N(5) | C(7) | C(8) | 113(1) | N(5) | C(7) | H(7) | 122.9 |
| C(8) | C(7) | H(7) | 123.5 | N(6) | C(8) | C(7) | 109(1) |
| N(6) | C(8) | H(8) | 122.8 | C(7) | C(8) | H(8) | 127.4 |
| N(7) | C(9) | C(10) | 105(1) | N(7) | C(9) | H(9) | 125.9 |
| C(10) | C(9) | H(9) | 127.6 | N(8) | C(10) | C(9) | 110(1) |
| N(8) | C(10) | H(10) | 123.3 | C(9) | C(10) | H(10) | 126.0 |
| N(5) | C(11) | N(6) | 107.6(8) | N(5) | C(11) | C(12) | 114.1(9) |
| N(6) | C(11) | C(12) | 138(1) | N(7) | C(12) | N(8) | 116(1) |
| N(7) | C(12) | C(11) | 116.3(10) | N(8) | C(12) | C(11) | 126(1) |
| N(9) | C(13) | C(14) | 108(1) | N(9) | C(13) | H(12) | 122.6 |
| C(14) | C(13) | H(12) | 128.8 | N(10) | C(14) | C(13) | 107(1) |
| N(10) | C(14) | H(13) | 124.6 | C(13) | C(14) | H(13) | 126.0 |
| N(11) | C(15) | C(16) | 106.8(9) | N(11) | C(15) | H(14) | 126.2 |
| C(16) | C(15) | H(14) | 126.8 | N(12) | C(16) | C(15) | 111(1) |
| N(12) | C(16) | H(15) | 119.8 | C(15) | C(16) | H(15) | 128.4 |
| N(9) | C(17) | N(10) | 114.7(9) | N(9) | C(17) | C(18) | 115.8(9) |
| N(10) | C(17) | C(18) | 129.2(9) | N(11) | C(18) | N(12) | 126(1) |
| N(11) | C(18) | C(17) | 106(1) | N(12) | C(18) | C(17) | 126(1) |

Table 4. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|-----------|-------|-------|-------|-----------|
| N(13) | C(19) | C(20) | 101.3(10) | N(13) | C(19) | H(17) | 128.8 |
| C(20) | C(19) | H(17) | 129.8 | N(14) | C(20) | C(19) | 108.2(10) |
| N(14) | C(20) | H(18) | 122.9 | C(19) | C(20) | H(18) | 128.9 |
| N(15) | C(21) | C(22) | 109(1) | N(15) | C(21) | H(19) | 129.7 |
| C(22) | C(21) | H(19) | 121.0 | N(16) | C(22) | C(21) | 108.2(10) |
| N(16) | C(22) | H(20) | 123.7 | C(21) | C(22) | H(20) | 126.6 |
| N(13) | C(23) | N(14) | 116.3(10) | N(13) | C(23) | C(24) | 120(1) |
| N(14) | C(23) | C(24) | 123.1(10) | N(15) | C(24) | N(16) | 109.9(10) |
| N(15) | C(24) | C(23) | 112.2(10) | N(16) | C(24) | C(23) | 137(1) |
| N(17) | C(25) | C(26) | 101.7(9) | N(17) | C(25) | H(22) | 129.5 |
| C(26) | C(25) | H(22) | 128.8 | N(18) | C(26) | C(25) | 110.5(10) |
| N(18) | C(26) | H(23) | 121.9 | C(25) | C(26) | H(23) | 127.2 |
| N(19) | C(27) | C(28) | 109.5(10) | N(19) | C(27) | H(24) | 127.0 |
| C(28) | C(27) | H(24) | 123.6 | N(20) | C(28) | C(27) | 111.4(10) |
| N(20) | C(28) | H(25) | 120.4 | C(27) | C(28) | H(25) | 128.0 |
| N(17) | C(29) | N(18) | 111.5(9) | N(17) | C(29) | C(30) | 113(1) |
| N(18) | C(29) | C(30) | 134(1) | N(19) | C(30) | N(20) | 113(1) |
| N(19) | C(30) | C(29) | 112.7(10) | N(20) | C(30) | C(29) | 132(1) |
| N(21) | C(31) | C(32) | 107(1) | N(21) | C(31) | H(27) | 132.8 |
| C(32) | C(31) | H(27) | 119.4 | N(22) | C(32) | C(31) | 107(1) |
| N(22) | C(32) | H(28) | 124.5 | C(31) | C(32) | H(28) | 125.8 |
| N(23) | C(33) | C(34) | 106.9(9) | N(23) | C(33) | H(29) | 123.7 |
| C(34) | C(33) | H(29) | 129.3 | N(24) | C(34) | C(33) | 106.9(9) |
| N(24) | C(34) | H(30) | 126.8 | C(33) | C(34) | H(30) | 126.0 |

Table 4. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|-----------|-------|-------|-------|----------|
| N(21) | C(35) | N(22) | 106.6(10) | N(21) | C(35) | C(36) | 118(1) |
| N(22) | C(35) | C(36) | 135(1) | N(23) | C(36) | N(24) | 100.3(7) |
| N(23) | C(36) | C(35) | 124.0(8) | N(24) | C(36) | C(35) | 135.7(9) |