Salicylaldimine Ruthenium Alkylidene Complexes: Metathesis Catalysts Tuned for Protic Solvents

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Figure 1S. Solid-state molecular structure of complex **7a**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are shown at 50% probability.



Figure 2S. Solid-state molecular structure of complex 7a. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are shown at 50% probability.

| Identification code | raines05 | |
|---|-----------------------------------|---------------------------------|
| Empirical formula | C43H45BrClN3ORu | |
| Formula weight | 836.25 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | $P\overline{I}$ | |
| Unit cell dimensions | a = 11.2903(8) Å | $\alpha = 107.0270(10)^{\circ}$ |
| | b = 11.3962(8) Å | $\beta = 90.5140(10)^{\circ}$ |
| | c = 16.3627(12) Å | $\gamma = 110.8190(10)^{\circ}$ |
| Volume | 1866.5(2) Å ³ | |
| Ζ | 2 | |
| Density (calculated) | 1.488 Mg/m^{3} | |
| Absorption coefficient | 1.600 mm^{-1} | |
| F(000) | 856 | |
| Crystal size | $0.36 \times 0.31 \times 0.30$ mm | m ³ |
| Theta range for data collection | 1.31 to 26.39° | |
| Index ranges | $-14 \le h \le 14, -14 \le k$ | $\leq 14, -20 \leq l \leq 20$ |
| Reflections collected | 27052 | |
| Independent reflections | 7597 [R(int) = 0.0252] | 2] |
| Completeness to theta = 26.39° | 99.4% | |
| Absorption correction | Multi-scan with SAD | ABS |
| Max. and min. transmission | 0.6454 and 0.5966 | 2 |
| Refinement method | Full-matrix least-squa | ares on F^2 |
| Data / restraints / parameters | 7597 / 0 / 459 | |
| Goodness-of-fit on F^2 | 1.079 | |
| Final <i>R</i> indices [<i>I</i> >2sigma(I)] | R1 = 0.0262, wR2 = 0 | 0.0662 |
| <i>R</i> indices (all data) | R1 = 0.0335, wR2 = 0 | 0.0739 |
| Largest diff. peak and hole | 0.925 and -0.396 e.Å | -3 |
| | | |

 Table S1. Crystal data and structure refinement of complex 7a.

| | x | У | Z | U(eq) |
|-----------------------------|--------------------|----------------------|--------------------|-----------------------|
| $\overline{\mathbf{Ru}(1)}$ | 6706(1) | 9153(1) | 2513(1) | 14(1) |
| Br(1) | 1145(1) | 2716(1) | 1665(1) | 26(1) |
| Cl(1) | 6017(1) | 7643(1) | 3327(1) | 22(1) |
| O(1) | 7410(1) | 10286(1) | 1727(1) | 16(1) |
| N(1) | 5202(2) | 7849(2) | 1528(1) | 16(1) |
| N(2) | 9405(2) | 9574(2) | 2856(1) | 17(1) |
| N(3) | 9121(2) | 11259(2) | 3741(1) | 17(1) |
| C(1) | 7012(2) | 10059(2) | 926(1) | 16(1) |
| C(2) | 7702(2) | 10975(2) | 510(2) | 19(1) |
| C(3) | 7386(2) | 10780(2) | -341(2) | 21(1) |
| C(4) | 6342(2) | 9662(2) | -841(2) | 21(1) |
| C(5) | 5635(2) | 8787(2) | -449(1) | 19(1) |
| C(6) | 5933(2) | 8943(2) | 429(1) | 16(1) |
| C(7) | 5125(2) | 7959(2) | 762(1) | 17(1) |
| C(8) | 4242(2) | 6665(2) | 1611(1) | 16(1) |
| C(9) | 3092(2) | 6684(2) | 1011(1) 1912(1) | 17(1) |
| C(10) | 2169(2) | 5496(2) | 1912(1) 1936(1) | 17(1) 18(1) |
| C(11) | 2409(2) 2417(2) | 4348(2) | 1668(1) | 19(1) |
| C(12) | 3561(2) | 4331(2) | 1391(1) | 19(1) |
| C(12) C(13) | 4499(2) | 5503(2) | 1367(1) | 17(1) |
| C(13) | 2844(2) | 7948(2) | 2219(2) | 21(1) |
| C(14) | 5779(2) | 5526(2) | 1100(2) | 21(1) 22(1) |
| C(16) | 8514(2) | 10075(2) | 3139(1) | 15(1) |
| C(10) | 10498(2) | 11565(2) | 3937(2) | 22(1) |
| C(17) | 10723(2) | 10503(2) | 3207(2) | 19(1) |
| C(10) | 8542(2) | 10303(2) 12092(2) | 4284(1) | 16(1) |
| C(20) | 8664(2) | 12092(2) 13280(2) | 4147(1) | 10(1) 18(1) |
| C(20) | 8110(2) | 13200(2) 14077(2) | 4685(2) | 20(1) |
| C(21) | 7442(2) | 13715(2) | 5338(2) | 20(1) |
| C(22) | 7365(2) | 12542(2) | 5468(1) | 20(1) 21(1) |
| C(24) | 7919(2) | 11715(2) | 4954(1) | 19(1) |
| C(25) | 9340(2) | 13679(2) | 3426(2) | 24(1) |
| C(26) | 6792(2) | 14561(2) | 5878(2) | 27(1) |
| C(20) | 7821(2) | 10450(2) | 5115(2) | 24(1) |
| C(28) | 9173(2) | 8281(2) | 2255(1) | 17(1) |
| C(29) | 8989(2) | 7224(2) | 2578(2) | 19(1) |
| C(30) | 8820(2) | 5994(2) | 1994(2) | 19(1) |
| C(31) | 8828(2) | 5790(2) | 1115(2) | 19(1) |
| C(32) | 9046(2) | 6860(2) | 819(2) | 19(1) |
| C(32) | 9246(2) | 8127(2) | 1378(2) | 19(1) 18(1) |
| C(34) | 8979(2) | 7388(2) | 3527(2) | 25(1) |
| C(35) | 8582(2) | 4424(2) | 504(2) | 25(1) 26(1) |
| C(36) | 9574(2) | 9273(2) | 1029(2) | 23(1) |
| C(37) | 5970(2) | 10202(2) | 3222(1) | 19(1) |
| C(38) | 5700(2) | 10202(2) 11372(2) | 3222(1) 3206(2) | 20(1) |
| C(30) | 6186(2) | 1272(2) 12122(2) | 2666(2) | 23(1) |
| C(40) | 5873(3) | 12132(2) 13216(3) | 2700(2) | 29(1) |
| C(41) | 5058(3) | 13554(3) | 3269(2) | $\frac{29(1)}{38(1)}$ |
| C(42) | <u>4575(3)</u> | 12827(3) | 3207(2) 3814(2) | 40(1) |
| C(-2) | 4808(2) | 12027(3) 11745(3) | 3790(2) | 30(1) |
| | 1070(2) | 117 (5) | 5790(2) | 50(1) |

Table S2. Atomic coordinates (×10⁴) and equivalent isotropic displacement parameters (Å² × 10³) of complex **7a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

 Table S3. Bond lengths [Å] and angles [°] of complex 7a.

| Ru(1)-C(37) | 1.838(2) | C(20)-C(25) | 1.505(3) |
|--|----------------------|--|----------------------|
| Ru(1)-C(16) | 2.032(2) | C(21)-C(22) | 1.389(3) |
| Ru(1)-O(1) | 2.0530(15) | C(21)-H(21) | 0.9500 |
| Ru(1)-N(1) | 2.1080(18) | C(22)-C(23) | 1.388(3) |
| Ru(1)-Cl(1) | 2.3976(6) | C(22)-C(26) | 1.506(3) |
| Br(1)-C(11) | 1.902(2) | C(23)-C(24) | 1.397(3) |
| O(1)-C(1) | 1.301(3) | C(23)-H(23) | 0.9500 |
| N(1)-C(7) | 1.301(3) | C(24)-C(27) | 1.506(3) |
| N(1)-C(8) | 1.444(3) | C(25)-H(25A) | 0.9800 |
| N(2)-C(16) | 1.347(3) | C(25)-H(25B) | 0.9800 |
| N(2)-C(28) | 1.442(3) | C(25)-H(25C) | 0.9800 |
| N(2)-C(18) | 1.475(3) | C(26)-H(26A) | 0.9800 |
| N(3)-C(16) | 1.346(3) | C(26)-H(26B) | 0.9800 |
| N(3)-C(19) | 1.441(3) | C(26)-H(26C) | 0.9800 |
| N(3)-C(17) | 1.477(3) | C(27)-H(27A) | 0.9800 |
| C(1)-C(2) | 1 417(3) | C(27)-H(27B) | 0 9800 |
| C(1) - C(6) | 1 428(3) | C(27)-H(27C) | 0 9800 |
| C(2)-C(3) | 1 367(3) | C(28)-C(33) | 1 400(3) |
| C(2)-H(2) | 0.9500 | C(28) - C(29) | 1.404(3) |
| C(3)-C(4) | 1 410(3) | C(29)-C(30) | 1 392(3) |
| C(3)-H(3) | 0.9500 | C(29)-C(34) | 1.5)2(3) |
| C(4)-C(5) | 1 364(3) | C(30)-C(31) | 1.388(3) |
| C(4)-H(4) | 0.9500 | C(30)-H(30) | 0.9500 |
| C(5)-C(6) | 1 417(3) | C(31)-C(32) | 1384(3) |
| C(5)-H(5) | 0.9500 | C(31)-C(35) | 1 509(3) |
| C(6)-C(7) | 1 423(3) | C(32)-C(33) | 1.509(3) 1 402(3) |
| C(7)-H(7) | 0.9500 | C(32)-E(33) | 0.9500 |
| C(8)-C(9) | 1 398(3) | C(32) - T(32) C(33) - C(36) | 1 505(3) |
| C(8)-C(13) | 1.000(0) | C(34)-H(34A) | 0.9800 |
| C(9)-C(10) | 1 396(3) | C(34)-H(34B) | 0.9800 |
| C(9)-C(14) | 1.507(3) | C(34)-H(34C) | 0.9800 |
| C(10)-C(11) | 1 381(3) | C(35)-H(35A) | 0.9800 |
| C(10)-E(11) | 0.9500 | C(35)-H(35R) | 0.9800 |
| C(11)-C(12) | 1 377(3) | C(35)-H(35C) | 0.9800 |
| C(12)-C(12) | 1 393(3) | C(36)-H(364) | 0.9800 |
| C(12) - C(13) C(12) - H(12) | 0.9500 | C(36) H(36R) | 0.9800 |
| $C(12)$ - $\Pi(12)$ C(13) $C(15)$ | 1 505(3) | C(36) H(36C) | 0.9800 |
| C(13)- $C(13)$ | 0.9800 | C(37) C(38) | 1.76(3) |
| C(14) - H(14R) C(14) + H(14R) | 0.9800 | C(37) - C(38) | 0.9500 |
| C(14) - H(14C) | 0.9800 | $C(37)^{-11}(37)$ C(38) C(30) | 1.308(A) |
| $C(14) - \Pi(14C)$ $C(15) - \Pi(15A)$ | 0.9800 | C(38) - C(39) | 1.390(4) 1.402(3) |
| C(15) H(15R) | 0.9800 | C(38)-C(43) | 1.402(3) 1.297(2) |
| C(15) - H(15C) | 0.9800 | C(39)-C(40) C(30) $H(30)$ | 1.587(5) |
| C(17) C(18) | 1 528(3) | $C(39)$ - $\Pi(39)$ C(40) $C(41)$ | 1.395(4) |
| C(17) + C(10) C(17) + C(17A) | 0.0000 | C(40) - C(41) C(40) - H(40) | 0.0500 |
| C(17) H(17R) | 0.9200 | $C(40) - \Pi(40)$ C(41) C(42) | 1 270(1) |
| C(18) H(18A) | 0.9900 | C(41) + C(42) | 0.0500 |
| C(10) - H(10A) C(12) - H(12D) | 0.9200 | $C(41)^{-11}(41)$ C(42) C(42) | 1 205(1) |
| $C(10) - \Pi(10D)$ C(10) C(20) | 0.7700 | C(42) - C(43) C(42) - U(43) | 0.0500 |
| C(17)- $C(20)C(10)$ $C(24)$ | 1.370(3) 1.200(2) | $C(42)$ - $\Pi(42)$ $C(42)$ $\Pi(42)$ | 0.9500 |
| C(20) C(21) | 1.377(3) 1.201(2) | C(+3)-11(+3) | 0.2500 |
| $(20)^{-}(21)$ | 1.371(3) | | |

| C(37)-Ru(1)-C(16) | 98.28(9) | C(8)-C(13)-C(15) | 120.8(2) |
|---|--------------------------|--|----------------------|
| C(37)-Ru(1)-O(1) | 98.70(9) | C(9)-C(14)-H(14A) | 109.5 |
| C(16)-Ru(1)-O(1) | 83.79(7) | C(9)-C(14)-H(14B) | 109.5 |
| C(37)-Ru(1)-N(1) | 103.07(8) | H(14A)-C(14)-H(14B) | 109.5 |
| C(16)-Ru(1)-N(1) | 158.34(8) | C(9)-C(14)-H(14C) | 109.5 |
| O(1)-Ru(1)-N(1) | 89.40(6) | H(14A)-C(14)-H(14C) | 109.5 |
| C(37)-Ru(1)-Cl(1) | 88.79(8) | H(14B)-C(14)-H(14C) | 109.5 |
| C(16)-Ru(1)-Cl(1) | 94.73(6) | C(13)-C(15)-H(15A) | 109.5 |
| O(1)-Ru(1)-Cl(1) | 172.50(4) | C(13)-C(15)-H(15B) | 109.5 |
| N(1)-Ru(1)-Cl(1) | 89.35(5) | H(15A)-C(15)-H(15B) | 109.5 |
| C(1)-O(1)-Ru(1) | 128.81(14) | C(13)-C(15)-H(15C) | 109.5 |
| C(7)-N(1)-C(8) | 113.62(18) | H(15A)-C(15)-H(15C) | 109.5 |
| C(7)-N(1)-Ru(1) | 123.27(15) | H(15B)-C(15)-H(15C) | 109.5 |
| C(8)-N(1)-Ru(1) | 122.74(14) | N(3)-C(16)-N(2) | 107.30(18) |
| C(16)-N(2)-C(28) | 126.34(18) | N(3)-C(16)-Ru(1) | 132.79(16) |
| C(16)-N(2)-C(18) | 113.45(18) | N(2)-C(16)-Ru(1) | 119.09(15) |
| C(28)-N(2)-C(18) | 120.19(17) | N(3)-C(17)-C(18) | 102.23(17) |
| C(16)-N(3)-C(19) | 126.97(18) | N(3)-C(17)-H(17A) | 111.3 |
| C(16)-N(3)-C(17) | 113.04(18) | C(18)-C(17)-H(17A) | 111.3 |
| C(19)-N(3)-C(17) | 119.04(17) | N(3)-C(17)-H(17B) | 111.3 |
| O(1)-C(1)-C(2) | 117.95(19) | C(18)-C(17)-H(17B) | 111.3 |
| O(1)-C(1)-C(6) | 124.8(2) | H(17A)-C(17)-H(17B) | 109.2 |
| C(2)-C(1)-C(6) | 117.2(2) | N(2)-C(18)-C(17) | 101.67(17) |
| C(3)-C(2)-C(1) | 121.8(2) | N(2)-C(18)-H(18A) | 111.4 |
| C(3)-C(2)-H(2) | 119.1 | C(17)-C(18)-H(18A) | 111.4 |
| C(1)-C(2)-H(2) | 119.1 | N(2)-C(18)-H(18B) | 111.4 |
| C(2)-C(3)-C(4) | 121.2(2) | C(17)-C(18)-H(18B) | 111.4 |
| C(2)-C(3)-H(3) | 119.4 | H(18A)-C(18)-H(18B) | 109.3 |
| C(4)-C(3)-H(3) | 119.4 | C(20)-C(19)-C(24) | 121.9(2) |
| C(5)-C(4)-C(3) | 118.2(2) | C(20)-C(19)-N(3) | 118.9(2) |
| C(5)-C(4)-H(4) | 120.9 | C(24)-C(19)-N(3) | 119.2(2) |
| C(3)-C(4)-H(4) | 120.9 | C(21)-C(20)-C(19) | 118.0(2) |
| C(4)-C(5)-C(6) | 122.6(2) | C(21)-C(20)-C(25) | 120.5(2) |
| C(4)-C(5)-H(5) | 118.7 | C(19)-C(20)-C(25) | 121.5(2) |
| C(6)-C(5)-H(5) | 118.7 | C(22)-C(21)-C(20) | 121.9(2) |
| C(5)-C(6)-C(7) | 117.2(2) | C(22)-C(21)-H(21) | 119.0 |
| C(5)-C(6)-C(1) | 119.0(2) | C(20)-C(21)-H(21) | 119.0 |
| V(1) - C(6) - C(1) | 123.8(2) | C(23)-C(22)-C(21) | 118.6(2) 120.7(2) |
| N(1)-C(7)-C(6) | 129.6(2) | C(23)-C(22)-C(26) | 120.7(2) |
| N(1)-C(7)-H(7) | 115.2 | C(21)-C(22)-C(20) C(22)-C(24) | 120.8(2) 121.8(2) |
| $C(0) - C(7) - \Pi(7)$ | 113.2 | C(22) - C(23) - C(24) | 121.0(2) |
| C(9) - C(8) - C(13) | 121.8(2) 120.70(10) | $C(22)-C(23)-\Pi(23)$ $C(24)-C(23)-\Pi(23)$ | 119.1 |
| C(9)-C(0)-N(1) C(12) C(8) N(1) | 120.70(19) 117.40(10) | $C(24)-C(25)-\Pi(25)$ C(23)-C(24)-C(10) | 119.1 117.8(2) |
| C(13)-C(8)-N(1) | 117.49(19) 118.2(2) | C(23) - C(24) - C(19) C(23) - C(24) - C(27) | 11/.0(2) 120.5(2) |
| C(10) - C(9) - C(8) | 118.3(2) 120.1(2) | C(23)-C(24)-C(27) | 120.3(2) 121.7(2) |
| C(10)- $C(9)$ - $C(14)$ | 120.1(2) 121.6(2) | C(19)-C(24)-C(27) C(20) C(25) H(25A) | 121.7(2) 100.5 |
| C(3)-C(3)-C(14) C(11) C(10) C(0) | 121.0(2) 110.6(2) | C(20) - C(25) - H(25R) C(20) - C(25) - H(25R) | 109.5 |
| C(11) - C(10) - C(9) C(11) - C(10) - H(10) | 119.0(2) | $U(20)-U(23)-\Pi(23D)$ U(25A) C(25) U(25B) | 109.5 |
| C(11)- $C(10)$ - $H(10)$ | 120.2 | $\Gamma(23A) - C(23) - \Pi(23B)$ $C(20) - C(25) - \Pi(25C)$ | 109.5 |
| C(9)- $C(10)$ - $H(10)C(12)$ $C(11)$ $C(10)$ | 120.2 122.3(2) | $U(20)-U(23)-\Pi(23U)$ U(25A) C(25) U(25C) | 109.5 |
| C(12)- $C(11)$ - $C(10)C(12)$ $C(11)$ Br(1) | 122.3(2) 117.85(17) | H(25R) - C(25) - H(25C) H(25R) - C(25) - H(25C) | 109.5 |
| C(10)- $C(11)$ -Br(1) | 119.80(17) | C(22)-C(23)-H(25C) | 109.5 |
| C(11) - C(12) - C(13) | 119 3(2) | C(22) - C(26) - H(26R) | 109.5 |
| C(11)-C(12)-H(12) | 120.4 | H(26A)-C(26)-H(26B) | 109.5 |
| C(13)-C(12)-H(12) | 120.4 | C(22)-C(26)-H(26D) | 109.5 |
| C(12)-C(13)-C(13) | 118 7(2) | H(26A)-C(26)-H(26C) | 109.5 |
| C(12)- $C(13)$ - $C(15)$ | 120 5(2) | H(26B)-C(26)-H(26C) | 109.5 |
| -() = () = () | | | |

| C(24)-C(27)-H(27B) 109.5 C(31)-C(35)-H(35C) 10 | 09.5 |
|---|-----------|
| $H(2\pi A) = G(2\pi) H(2\pi B)$ 100 f $H(2\pi A) = G(2\pi B) H(2\pi B)$ | 00 5 |
| H(2/A)-C(2/)-H(2/B) 109.5 $H(35A)-C(35)-H(35C)$ 10 | 09.5 |
| C(24)-C(27)-H(27C) 109.5 H(35B)-C(35)-H(35C) 10 | 09.5 |
| H(27A)-C(27)-H(27C) 109.5 C(33)-C(36)-H(36A) 10 | 09.5 |
| H(27B)-C(27)-H(27C) 109.5 C(33)-C(36)-H(36B) 10 | 09.5 |
| C(33)-C(28)-C(29) 121.4(2) H(36A)-C(36)-H(36B) 10 | 09.5 |
| C(33)-C(28)-N(2) 119.8(2) C(33)-C(36)-H(36C) 10 | 09.5 |
| C(29)-C(28)-N(2) 118.6(2) H(36A)-C(36)-H(36C) 10 | 09.5 |
| C(30)-C(29)-C(28) 118.0(2) H(36B)-C(36)-H(36C) 10 | 09.5 |
| C(30)-C(29)-C(34) 119.8(2) C(38)-C(37)-Ru(1) 13 | 34.46(18) |
| C(28)-C(29)-C(34) 122.2(2) C(38)-C(37)-H(37) 11 | 12.8 |
| C(31)-C(30)-C(29) 122.2(2) Ru(1)-C(37)-H(37) 11 | 12.8 |
| C(31)-C(30)-H(30) 118.9 C(39)-C(38)-C(43) 11 | 18.1(2) |
| C(29)-C(30)-H(30) 118.9 C(39)-C(38)-C(37) 12 | 25.3(2) |
| C(32)-C(31)-C(30) 118.5(2) $C(43)-C(38)-C(37)$ 11 | 16.6(2) |
| C(32)-C(31)-C(35) 121.4(2) $C(40)-C(39)-C(38)$ 12 | 20.9(2) |
| C(30)-C(31)-C(35) 120.1(2) C(40)-C(39)-H(39) 11 | 19.5 |
| C(31)-C(32)-C(33) 121.9(2) C(38)-C(39)-H(39) 11 | 19.5 |
| C(31)-C(32)-H(32) 119.0 C(41)-C(40)-C(39) 12 | 20.2(3) |
| C(33)-C(32)-H(32) 119.0 C(41)-C(40)-H(40) 11 | 19.9 |
| C(28)-C(33)-C(32) 117.9(2) C(39)-C(40)-H(40) 11 | 19.9 |
| C(28)-C(33)-C(36) 122.4(2) C(42)-C(41)-C(40) 11 | 19.9(3) |
| C(32)-C(33)-C(36) 119.6(2) C(42)-C(41)-H(41) 12 | 20.0 |
| C(29)-C(34)-H(34A) 109.5 C(40)-C(41)-H(41) 12 | 20.0 |
| C(29)-C(34)-H(34B) 109.5 C(41)-C(42)-C(43) 12 | 20.1(3) |
| H(34A)-C(34)-H(34B) 109.5 C(41)-C(42)-H(42) 11 | 19.9 |
| C(29)-C(34)-H(34C) 109.5 C(43)-C(42)-H(42) 11 | 19.9 |
| H(34A)-C(34)-H(34C) 109.5 C(42)-C(43)-C(38) 12 | 20.7(3) |
| H(34B)-C(34)-H(34C) 109.5 C(42)-C(43)-H(43) 11 | 19.7 |
| C(31)-C(35)-H(35A) 109.5 C(38)-C(43)-H(43) 11 | 19.7 |
| C(31)-C(35)-H(35B) 109.5 | |

Symmetry transformations were used to generate equivalent atoms.

| | 7.1 | | 22 | | 12 | 12 |
|----------------|-----------------------|-----------------------|-----------------------|---------------------|----------------------|----------------------|
| | U^{I1} | U^{22} | U^{33} | U^{23} | U^{13} | U^{12} |
| | | | | | | |
| Ru(1) | 14(1) | 10(1) | 15(1) | 2(1) | 2(1) | 4(1) |
| Br(1) | 26(1) | 17(1) | 29(1) | 7(1) | 8(1) | -1(1) |
| Cl(1) | 25(1) | 16(1) | 21(1) | 7(1) | 2(1) | 3(1) |
| O(1) | 16(1) | 13(1) | 17(1) | 4(1) | 2(1) | 3(1) |
| N(1) | 15(1) | 12(1) | 18(1) | 3(1) | 3(1) | 5(1) |
| N(2) | 15(1) | 12(1) | 20(1) | 1(1) | 1(1) | 4(1) |
| N(3) | 16(1) | 14(1) | 18(1) | 1(1) | 1(1) | 6(1) |
| C(1) | 17(1) | 15(1) | 18(1) | 3(1) | 3(1) | 10(1) |
| C(2) | 19(1) | 14(1) | 25(1) | 6(1) | 3(1) | 6(1) |
| C(3) | 21(1) | 20(1) | 26(1) | 13(1) | 8(1) | 8(1) |
| C(4) | 25(1) | 21(1) | 18(1) | 6(1) | 3(1) | 11(1) |
| C(5) | 22(1) | 14(1) | 18(1) | 1(1) | 1(1) | 7(1) |
| C(6) | 17(1) | 14(1) | 19(1) | 4(1) | 4(1) | 9(1) |
| C(7) | 16(1) | 13(1) | 20(1) | 1(1) | 2(1) | 7(1) |
| C(8) | 17(1) | 12(1) | 15(1) | 2(1) | -1(1) | 2(1) |
| C(9) | 17(1) | 18(1) | 15(1) | 5(1) | 1(1) | 6(1) |
| C(10) | 16(1) | 21(1) | 17(1) | 6(1) | 5(1) | 6(1) |
| C(11) | 20(1) | 13(1) | 17(1) | 4(1) | 1(1) | -2(1) |
| C(12) | 20(1) 21(1) | 12(1) | 19(1) | 2(1) | 2(1) | 5(1) |
| C(12) C(13) | 16(1) | 12(1) 16(1) | 19(1) 18(1) | $\frac{2(1)}{3(1)}$ | 2(1) 2(1) | 5(1) |
| C(13) C(14) | 22(1) | 18(1) | 25(1) | $\frac{3(1)}{8(1)}$ | $\frac{2(1)}{6(1)}$ | $\frac{3(1)}{8(1)}$ |
| C(14) | 19(1) | 16(1) | 29(1) | 2(1) | $\frac{0(1)}{4(1)}$ | 7(1) |
| C(15) | 20(1) | 10(1) 11(1) | $\frac{25(1)}{15(1)}$ | 5(1) | $\frac{1}{1}$ | 6(1) |
| C(10) C(17) | 18(1) | 10(1) | 25(1) | $\frac{3(1)}{1(1)}$ | -3(1) | 7(1) |
| C(17) C(18) | 16(1) | 15(1) 16(1) | 23(1) 22(1) | 2(1) | -3(1) | 5(1) |
| C(10) | 18(1) | 13(1) | $\frac{22(1)}{14(1)}$ | $\frac{2(1)}{1(1)}$ | -1(1) | 5(1) |
| C(19) | 10(1) | 13(1) 14(1) | 17(1) | -1(1) 3(1) | -1(1) 1(1) | $\frac{J(1)}{A(1)}$ |
| C(20) | $\frac{19(1)}{23(1)}$ | 14(1) 12(1) | $\frac{1}{(1)}$ | $\frac{3(1)}{2(1)}$ | -1(1) | 7(1) |
| C(21) C(22) | 23(1) 22(1) | 12(1) 18(1) | $\frac{22(1)}{10(1)}$ | 2(1) 2(1) | 2(1) | $\frac{7(1)}{8(1)}$ |
| C(22) C(23) | 22(1) 24(1) | 10(1) 21(1) | 19(1) 16(1) | $\frac{2(1)}{5(1)}$ | $\frac{2(1)}{4(1)}$ | 6(1) |
| C(23) | 24(1) 20(1) | $\frac{21(1)}{15(1)}$ | 10(1) 17(1) | $\frac{3(1)}{4(1)}$ | $\frac{4(1)}{2(1)}$ | $\frac{0(1)}{4(1)}$ |
| C(24) | 20(1) | 13(1) 22(1) | $\frac{1}{(1)}$ | $\frac{4(1)}{8(1)}$ | -2(1) | 4(1) |
| C(25) | $\frac{29(1)}{22(1)}$ | 22(1) 22(1) | 22(1) 20(1) | 6(1) | $\frac{7(1)}{10(1)}$ | 11(1) 14(1) |
| C(20) C(27) | 33(1) 30(1) | $\frac{22(1)}{10(1)}$ | 29(1) 21(1) | $\frac{0(1)}{7(1)}$ | 10(1) | $\frac{14(1)}{9(1)}$ |
| C(27) | 30(1) | 19(1) 14(1) | 21(1) 21(1) | $\frac{7(1)}{2(1)}$ | 1(1) 2(1) | 6(1) |
| C(20) | 13(1) 17(1) | 14(1) 10(1) | 21(1) 22(1) | $\frac{2(1)}{6(1)}$ | 2(1) 2(1) | 0(1) |
| C(29) | $\frac{1}{(1)}$ | 19(1) 14(1) | 22(1) 26(1) | 0(1) 8(1) | $\frac{2(1)}{4(1)}$ | $\frac{0(1)}{7(1)}$ |
| C(30) | 20(1) | 14(1) 15(1) | 20(1) | 0(1) | 4(1) | 7(1) |
| C(31) | 10(1) | 13(1) 10(1) | 23(1) 10(1) | 3(1) | 4(1) | 7(1) |
| C(32) | 19(1) 15(1) | 19(1) | 19(1) | 4(1) | 5(1) | 9(1) |
| C(33) | 15(1) | 10(1) | 23(1) | 0(1) | 3(1) | (1) |
| C(34) | 33(1) | 23(1) | 21(1) 21(1) | $\frac{7(1)}{2(1)}$ | 2(1) | 13(1) |
| C(35) | 29(1) | 15(1) | 31(1) | 3(1) | 6(1) | 8(1) |
| C(36) | 29(1) | 20(1) | 26(1) | 9(1) | $\prod_{i=1}^{i}$ | 12(1) |
| C(37) | $\frac{1}{(1)}$ | 16(1) | 18(1) | I(1) | 0(1) | 4(1) |
| C(38) | 18(1) | $\frac{1}{(1)}$ | 22(1) | -1(1) | -1(1) | /(1) |
| C(39) | 26(1) | 19(1) | 21(1) | 1(1) | U(1) | $\Pi(1)$ |
| C(40) | 57(1) | 24(1) | 28(1) | 6(1) | 1(1) | 16(1) |
| C(41) | 43(2) | 33(2) | 47(2) | 9(1) | (1) | 29(1) |
| C(42) | 42(2) | 38(2) | 52(2) | 11(1) | 20(1) | 30(1) |
| C(43) | 27(1) | 28(1) | 37(2) | 8(1) | 11(1) | 14(1) |
| | | | | | | |

Table S4. Anisotropic displacement parameters (Å² × 10³) of complex **7a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2h k a^* b^* U^{12}]$.

| | x | у | Z | U(eq) |
|--------------------------|--------------|---------|-------|-----------|
| H(2) | 8404 | 11745 | 831 | 23 |
| H(3) | 7878 | 11410 | -600 | 25 |
| H(4) | 6137 | 9521 | -1435 | 25 |
| H(5) | 4916 | 8044 | -777 | 23 |
| H(7) | 4426 | 7283 | 366 | 20 |
| H(10) | 1377 | 5477 | 2134 | 22 |
| H(12) | 3709 | 3528 | 1223 | 22 |
| H(12) $H(14\Delta)$ | 3345 | 8493 | 2783 | 32 |
| H(14R) | 1033 | 7738 | 2785 | 32 |
| H(14C) | 2004 | 8/35 | 1805 | 32 |
| H(14C) H(15A) | 5707 | 4627 | 070 | 32 |
| $\Pi(1SA)$ | 5/9/ | 4057 | 970 | 22 |
| H(15B) | 0451 5022 | 0144 | 15/5 | <i>33</i> |
| H(15C) | 5922 | 5815 | 288 | 33 |
| H(1/A) | 10693 | 11489 | 4507 | 27 |
| H(17B) | 11020 | 12464 | 3927 | 27 |
| H(18A) | 11171 | 10875 | 2769 | 23 |
| H(18B) | 11220 | 10073 | 3427 | 23 |
| H(21) | 8191 | 14893 | 4604 | 23 |
| H(23) | 6924 | 12295 | 5920 | 25 |
| H(25A) | 9099 | 14369 | 3314 | 35 |
| H(25B) | 9095 | 12908 | 2905 | 35 |
| H(25C) | 10265 | 14021 | 3590 | 35 |
| H(26A) | 6128 | 14027 | 6146 | 41 |
| H(26B) | 6403 | 14906 | 5513 | 41 |
| H(26C) | 7422 | 15301 | 6329 | 41 |
| H(27A) | 7523 | 10452 | 5676 | 35 |
| H(27B) | 8663 | 10383 | 5113 | 35 |
| H(27C) | 7215 | 9693 | 4661 | 35 |
| H(30) | 8694 | 5269 | 2203 | 23 |
| H(32) | 9060 | 6731 | 219 | 22 |
| H(34A) | 8254 | 6660 | 3609 | 37 |
| H(34R) | 8901 | 8233 | 3829 | 37 |
| H(34C) | 9777 | 7379 | 3761 | 37 |
| $H(35\Delta)$ | 8468 | 4423 | _91 | 30 |
| H(35R) | 7807 | 3788 | 621 | 30 |
| H(35D) | 0310 | J 1 7 5 | 585 | 30 |
| $\Pi(33C)$ $\Pi(26A)$ | 9310 | 41/3 | 1400 | 39 |
| $\Pi(30A)$ | 9507 | 9937 | 1400 | 33 25 |
| П(30В) Ц(26С) | 9132 | 890/ | 444 | 33 25 |
| H(30C) | 10499 | 9642 | 101/ | 55 |
| H(3/) | 5/03 | 9930 | 3708 | 22 |
| H(39) | 6739 | 11903 | 2269 | 27 |
| H(40) | 6218 | 13727 | 2332 | 35 |
| H(41) | 4833 | 14287 | 3283 | 46 |
| H(42) | 4020 | 13063 | 4206 | 48 |
| H(43) | 4571 | 11256 | 4173 | 36 |

| Table S5. Hydrogen coordinates (×10 ⁴) and isotropic | displacement parameters (Å ² × 10 ³) |
|---|---|
| of complex 7a. | |

 Table S6. Torsion angles [°] of complex 7a.

| $\begin{array}{llllllllllllllllllllllllllllllllllll$ | $\overline{C(37)}$ -Ru(1)-O(1)-C(1) | -108.13(18) | C(18)-N(2)-C(16)-Ru(1) | 164.69(15) |
|--|---|-------------|---|------------------------|
| $\begin{split} \widehat{N}(h) = \widehat{N}(h) = \widehat{V}(h) = (1) - (1$ | C(16)-Ru(1)-O(1)-C(1) | 154.40(18) | C(37)-Ru(1)-C(16)-N(3) | -15.3(2) |
| $\begin{array}{cccc} (i_1) : Ru(1) - O(1) - O(1) \\ (i_1) : Ru(1) - N(1) - O(1) \\ (i_2) : Ru(1) - N(1) - O(1) \\ (i_1) : Ru(1) - N(1) - O(1) \\ (i_2) : Ru(1) - N(1) - O(1) \\ (i_1) : Ru(1) - O(1) - O(1) \\ (i_1) : Ru(1) - O(1) - O(1) \\ (i_1) : Ru(1) - O(1) - O(1) \\ (i_1) : Ru(1) - N(1) - O(1) \\ (i_1) : Ru(1) - N(1) - O(1) \\ (i_1) : Ru(1) - O(1) - O(1) \\ (i_1) : Ru$ | N(1)-Ru(1)-O(1)-C(1) | -5.00(17) | O(1)-Ru(1)-C(16)-N(3) | 82.6(2) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | Cl(1)-Ru(1)-O(1)-C(1) | 75 4(4) | N(1)-Ru(1)-C(16)-N(3) | 154 99(19) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(37)-Ru(1)-N(1)-C(7) | 104 10(18) | Cl(1)-Ru(1)-C(16)-N(3) | -1048(2) |
| $\begin{array}{ccccc} 0(1) = R(1)^{N}(1) - C(7)^{'} & 5 \ 31(17)^{'} & 0(1) + R(1)^{-}(C16)^{N}(2)^{'} & 485.55(17)^{'} \\ C(1) + R(1) - N(1) - C(7)^{'} & 1-67.29(17)^{'} & N(1) + R(1)^{-}(C16)^{-}N(2)^{'} & 4-3.2(3)^{'} \\ C(1) + R(1) - N(1) - C(8)^{'} & 43.25(17)^{'} & C(1) + R(1)^{-}(C16)^{-}N(2)^{'} & 87.80(19)^{'} \\ C(1) + R(1) - N(1) - C(8)^{'} & 106.6(2)^{'} & C(10)^{-}N(2)^{-}C(18)^{'} & -17.80(19)^{'} \\ C(1) + R(1) - N(1) - C(8)^{'} & 5.35(15)^{'} & C(10) - N(2) - C(18)^{'} - C(17)^{'} & -167.92(19)^{'} \\ R(1) - 0(1) - C(1) - C(2)^{'} & -17.19(14)^{'} & C(22) - N(2) - C(18)^{'} - C(17)^{'} & -167.92(19)^{'} \\ R(1) - 0(1) - C(1) - C(2)^{'} & -2.5(3)^{'} & C(17)^{-}N(6)^{'} - C(20)^{'} & 81.6(3)^{'} \\ C(1) - C(2) - C(3)^{'} & -2.5(3)^{'} & C(17)^{-}N(6)^{'} - C(20)^{'} & 81.6(3)^{'} \\ C(2) - C(3) - C(4)^{'} & 0.8(4)^{'} & C(10)^{-}N(3)^{-}C(19)^{-}C(20)^{'} & 81.6(3)^{'} \\ C(2) - C(3) - C(4)^{'} & 0.8(4)^{'} & C(10)^{-}N(3)^{-}C(19)^{-}C(20)^{'} & 81.6(3)^{'} \\ C(2) - C(3) - C(4)^{'} & 0.8(4)^{'} & C(10)^{-}N(3)^{-}C(19)^{-}C(20)^{'} & 21.10^{'} \\ C(2) - C(3) - C(4)^{'} & 0.8(4)^{'} & C(10)^{-}N(3)^{-}C(19)^{-}C(20)^{'} & 21.13^{'} \\ C(2) - C(3) - C(4)^{'} & 0.13^{'} & C(2)^{-}C(2)^{'} & (21)^{'} & -179.28(19)^{'} \\ C(4) - C(5) - C(6)^{'} & -177.4(2)^{'} & N(3)^{-}C(19)^{-}C(20)^{-}C(21)^{'} & -179.8(2)^{'} \\ C(1) - C(6)^{-}C(7)^{'} & 2.5(3)^{'} & C(22)^{-}C(22)^{-}C(23)^{'} & 2.1(3)^{'} \\ C(2) - C(1)^{-}C(6)^{'} & -177.4(2)^{'} & N(3)^{-}C(19)^{-}C(20)^{-}C(21)^{'} & -179.8(2)^{'} \\ C(1) - C(1)^{-}C(6)^{'} & -178.2(2)^{'} & C(20)^{-}C(21)^{-}C(22)^{'} & -179.8(2)^{'} \\ C(1) - C(1)^{-}C(6)^{'} & -178.2(2)^{'} & C(20)^{-}C(21)^{-}C(22)^{'} & -179.8(2)^{'} \\ C(1) - C(1)^{-}C(6)^{'} & -177.4(2)^{'} & N(3)^{'} & C(22)^{-}C(23)^{'} & -179.9(1)^{'} \\ C(2) - C(1)^{-}C(6)^{'} & -177.4(2)^{'} & N(3)^{'} & C(22)^{-}C(23)^{'} & -179.8(2)^{'} \\ C(1) - C(1)^{-}C(6)^{'} & -178.2(2)^{'} & C(20)^{-}C(21)^{-}C(22)^{'} & -179.8(2)^{'} \\ C(1) - C(1)^{-}C(6)^{'} & -178.8(2)^{'} & -177.8(2)^{'} \\ C(1) - C(1)^{-}C(6)^{'} & -178.8(2)^{'} &$ | C(16)-Ru(1)-N(1)-C(7) | -66 1(3) | C(37)-Ru(1)-C(16)-N(2) | 17652(17) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | O(1)-Ru(1)-N(1)-C(7) | 531(17) | O(1)-Ru(1)-C(16)-N(2) | -85.55(17) |
| $\begin{array}{c} C(37) - Ru(1) - V(1) - C(3) & -R3 - 25(17) & C(1) - Ru(1) - V(1) - C(1) - V(1) & -V(1) - V(1) \\ C(10) - Ru(1) - V(1) - C(8) & 106.6(2) & C(10) - N(3) - C(17) - C(18) & 112.4(3) \\ O(1) - Ru(1) - V(1) - C(8) & 5.35(15) & C(16) - N(2) - C(18) - C(17) & -178.00(19) \\ C(10) - Ru(1) - V(1) - C(8) & 5.35(15) & C(16) - N(2) - C(18) - C(17) & -167.92(19) \\ Ru(1) - O(1) - C(1) - C(6) & 2.7(3) & N(3) - C(17) - C(18) - N(2) & -110.3(3) \\ C(10) - C(1) - C(2) - C(3) & -2.5(3) & C(17) - N(3) - C(19) - C(20) & 81.6(3) \\ C(1) - C(2) - C(3) & -2.5(3) & C(17) - N(3) - C(19) - C(20) & 81.6(3) \\ C(1) - C(2) - C(3) & -2.5(3) & C(17) - N(3) - C(19) - C(20) & 81.6(3) \\ C(2) - C(3) - C(4) & 0.8(4) & C(16) - N(3) - C(19) - C(20) & -19.8(3) \\ C(3) - C(4) - C(5) - C(6) & -1.8(3) & C(24) - C(19) - C(20) & -19.8(3) \\ C(3) - C(4) - C(5) - C(6) & -1.8(3) & C(24) - C(19) - C(20) & -179.28(19) \\ C(4) - C(5) - C(6) - (7) & -179.7(2) & N(3) - C(19) - C(20) - C(21) & -19.8(2) \\ O(1) - C(1) - C(6) - C(7) & -179.7(2) & N(3) - C(19) - C(20) - C(21) & -19.8(2) \\ O(1) - C(1) - C(6) - C(7) & 2.5(3) & C(25) - C(20) - C(21) - C(22) & -0.6(3) \\ O(1) - C(1) - C(6) - C(7) & 2.5(3) & C(25) - C(20) - C(21) - C(22) & -0.6(3) \\ O(1) - C(1) - C(6) - C(7) & 2.5(3) & C(21) - C(22) - C(23) & 2.1(3) \\ C(2) - C(1) - C(6) - C(7) & 2.5(3) & C(21) - C(22) - C(23) & -1.2(3) \\ C(2) - C(1) - C(6) - (7) - N(1) & -1.7(4) & C(22) - C(23) - C(24) & -1.2(3) \\ C(5) - C(6) - C(7) - N(1) & -1.7(4) & C(22) - C(23) - C(24) & -1.2(3) \\ C(5) - C(6) - C(7) - N(1) & -1.7(4) & C(22) - C(23) - C(24) & -1.2(3) \\ C(5) - C(6) - C(7) - N(1) & -1.7(4) & C(22) - C(23) - C(24) & -1.2(3) \\ C(5) - C(6) - C(7) - N(1) & -1.7(4) & C(22) - C(23) - C(24) & -1.7(3) \\ C(7) - N(1) - C(8) - C(9) & -9.90(19) & 0.16) - N(2) - C(23) - C(24) - C(27) & -178.3(2) \\ C(1) - C(1) - C(1) & -1.8(3) & N(2) - C(28) - C(29) - C(23) & -1.7(3) \\ C(7) - N(1) - C(8) - C(1) & -1.78.5(2) & C(20) - C(23) - C(24) - C(27) & -178.3(2) \\ C(1) - C(1) - C(1) & -1.78.10(16) & C(33) - C(28) - C(29) - C(30) & -177.3(2) \\ N(1) - C$ | Cl(1)-Ru(1)-N(1)-C(7) | -16729(17) | N(1)-Ru(1)-C(16)-N(2) | -132(3) |
| $\begin{array}{c} C(16)-Ru(1)+V(1)-C(18) & 106.6(2) & C(16)-V(3)-C(18) & 12.4(3) \\ O(1)-Ru(1)+V(1)-C(18) & 177.96(16) & C(19)-V(3)-C(17)-C(18) & 178.00(19) \\ C(1)-Ru(1)-V(1)-C(2) & 177.9(16) & C(19)-V(2)-C(18)-C(17) & 13.4(2) \\ Ru(1)-O(1)-C(1)-C(2) & -177.19(14) & C(28)-V(2)-C(18)-C(17) & 167.92(19) \\ Ru(1)-O(1)-C(1)-C(2) & -177.19(14) & C(28)-V(2)-C(19)-C(20) & 11.6(3) \\ C(1)-C(2)-C(3) & 1-69(2) & C(16)-V(3)-C(19)-C(20) & 11.6(3) \\ C(1)-C(2)-C(3) & -2.5(3) & C(17)-V(3)-C(19)-C(20) & 11.6(3) \\ C(2)-C(3)-C(4)-C(5) & 1.3(3) & C(17)-V(3)-C(19)-C(24) & -2.5(3) \\ C(2)-C(3)-C(4)-C(5) & 1.3(3) & C(17)-V(3)-C(19)-C(24) & -2.5(3) \\ C(3)-C(4)-C(5)-C(6) & -1.8(3) & C(24)-C(19)-C(20)-C(21) & -1.8(3) \\ C(4)-C(5)-C(6)-C(7) & -179.7(2) & N(3)-C(19)-C(20)-C(21) & -1.8(3) \\ C(2)-C(3)-C(4)-C(5) & 2.0(3) & C(2)-C(2)-C(22) & -0.6(3) \\ C(1)-C(1)-C(6)-C(5) & 2.0(3) & C(19)-C(20)-C(25) & 2.4(3) \\ C(2)-C(1)-C(6)-C(7) & -178.2(2) & C(20)-C(21)-C(22) & -176.6(2) \\ Ru(1)-N(1)-C(7)-C(6) & -13.3(3) & C(2)-C(2)-C(22)-C(23) & 2.1(3) \\ C(8)-N(1)-C(7)-C(6) & -176.5(2) & C(20)-C(21)-C(22) & -176.6(2) \\ Ru(1)-N(1)-C(7)-C(6) & -176.5(2) & C(20)-C(21)-C(22)-C(23) & 2.1(3) \\ C(3)-C(6)-C(7)-N(1) & 178.1(2) & C(26)-C(23)-C(24) & -1.2(3) \\ C(3)-C(6)-C(7)-N(1) & -1.7(4) & C(22)-C(23)-C(24) & -1.2(3) \\ C(5)-C(6)-C(7)-N(1) & -1.78.2(2) & C(20)-C(21)-C(22) & -2.7(3) \\ C(1)-C(6)-C(7) & -1.78.3(2) & C(20)-C(21)-C(22) & -2.7(3) \\ C(1)-C(6)-C(7) & -1.78.3(2) & C(20)-C(21)-C(22) & -2.7(3) \\ C(1)-C(6)-C(7)-N(1) & -1.78.1(2) & C(26)-C(23)-C(24) & -1.2(3) \\ C(3)-C(4)-C(9)-C(14) & 177.9(2) & C(3)-C(23)-C(24)-C(23) & -1.78.8(2) \\ Ru(1)-N(1)-C(8)-C(13) & -88.5(2) & C(20)-C(21)-C(22) & -2.7(3) \\ C(7)-N(1)-C(8)-C(13) & -88.5(2) & C(20)-C(21)-C(22) & -2.7(3) \\ C(7)-N(1)-C(8)-C(13) & -88.5(2) & C(20)-C(21)-C(23) & -2.7(3) \\ C(7)-N(1)-C(8)-C(13) & -88.5(2) & C(20)-C(23)-C(24) & -2.7(3) \\ C(1)-C(1)-C(1) & -1.78.10(16) & C(3)-C(23)-C(23) & -1.77.3(2) \\ C(9)-C(1)-C(1) & -1.78.10(16) & C(3)-C(23)-C(23) & -1.77.3(2) \\ C(9)-C(1)-C(1) & -1.78.10(16) & C(3)-C(23)-C(23) & -1.77.3(2) \\ C(9)-$ | C(37)-Ru(1)-N(1)-C(8) | -83.25(17) | $C_{1}(1) - R_{1}(1) - C_{1}(1) - N_{2}(2)$ | 87.06(16) |
| $\begin{array}{c} C(1) F(1) F(1) F(1) C(1) \\ (C(1) F(1) F(1) F(1) \\ (C(1) F(1) F(1) F(1) \\ (C(1) F$ | C(16)-Ru(1)-N(1)-C(8) | 106.6(2) | C(16)-N(3)-C(17)-C(18) | 124(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | O(1)-Ru(1)-N(1)-C(8) | 177 96(16) | C(19)-N(3)-C(17)-C(18) | -178.00(19) |
| $ \begin{array}{c} {\rm Ru}(1) - {\rm O}(1) - {\rm C}(1) - {\rm C}(2) & -177.19(14) & {\rm C}(28) - {\rm RU}(17) & -167.92(19) \\ {\rm Ru}(1) - {\rm O}(1) - {\rm C}(1) - {\rm C}(2) & -117.19(14) & {\rm C}(28) - {\rm RU}(17) & -167.92(19) \\ {\rm Ru}(1) - {\rm O}(1) - {\rm C}(2) - {\rm C}(3) & -2.5(3) & {\rm C}(17) - {\rm C}(18) - {\rm RO}(2) & 81.6(3) \\ {\rm C}(1) - {\rm C}(2) - {\rm C}(3) & -2.5(3) & {\rm C}(17) - {\rm N}(3) - {\rm C}(19) - {\rm C}(20) & 81.6(3) \\ {\rm C}(1) - {\rm C}(2) - {\rm C}(3) - {\rm C}(4) & 0.8(4) & {\rm C}(16) - {\rm N}(3) - {\rm C}(19) - {\rm C}(24) & -95.9(3) \\ {\rm C}(3) - {\rm C}(4) - {\rm C}(5) - {\rm C}(6) & -1.8(3) & {\rm C}(17) - {\rm N}(3) - {\rm C}(19) - {\rm C}(20) - {\rm C}(21) & -1.8(3) \\ {\rm C}(2) - {\rm C}(3) - {\rm C}(4) - {\rm C}(5) - {\rm C}(6) & -1.8(3) & {\rm C}(19) - {\rm C}(20) - {\rm C}(21) & -1.8(3) \\ {\rm C}(4) - {\rm C}(5) - {\rm C}(6) - {\rm C}(1) & 0.1(3) & {\rm C}(24) - {\rm C}(19) - {\rm C}(20) - {\rm C}(21) & -1.8(3) \\ {\rm C}(4) - {\rm C}(5) - {\rm C}(6) - {\rm C}(1) & 0.1(3) & {\rm C}(19) - {\rm C}(20) - {\rm C}(21) & -1.78.2(2) \\ {\rm O}(1) - {\rm C}(1) - {\rm C}(6) - {\rm C}(5) & -1.77.4(2) & {\rm N}(3) - {\rm C}(19) - {\rm C}(20) - {\rm C}(22) & -0.6(3) \\ {\rm O}(1) - {\rm C}(1) - {\rm C}(6) - {\rm C}(5) & -1.77.8(2) & {\rm C}(20) - {\rm C}(21) - {\rm C}(22) - {\rm C}(23) & -1.78.8(2) \\ {\rm C}(2) - {\rm C}(1) - {\rm C}(6) - {\rm C}(7) & 2.5(3) & {\rm C}(2) - {\rm C}(22) - {\rm C}(23) & -1.78.8(2) \\ {\rm C}(2) - {\rm C}(1) - {\rm C}(6) - {\rm C}(7) & 1.78.2(2) & {\rm C}(20) - {\rm C}(21) - {\rm C}(22) - {\rm C}(23) & -1.77.8(2) \\ {\rm C}(2) - {\rm C}(1) - {\rm C}(6) - {\rm C}(7) & 1.78.1(2) & {\rm C}(26) - {\rm C}(22) - {\rm C}(23) & -177.8(2) \\ {\rm C}(1) - {\rm C}(6) - {\rm C}(7) + {\rm N}(1) & 1.78.1(2) & {\rm C}(26) - {\rm C}(22) - {\rm C}(23) & -179.90(19) \\ {\rm C}(1) - {\rm C}(6) - {\rm C}(7) + {\rm N}(1) & 1.78.1(2) & {\rm C}(26) - {\rm C}(22) - {\rm C}(23) & -179.90(19) \\ {\rm R}(1) - {\rm N}(1) - {\rm C}(8) - {\rm C}(9) & 92.9(2) & {\rm C}(20) - {\rm C}(19) - {\rm C}(24) - {\rm C}(23) & -179.90(19) \\ {\rm R}(1) - {\rm N}(1) - {\rm C}(8) - {\rm C}(9) & 92.9(2) & {\rm C}(20) - {\rm C}(19) - {\rm C}(24) - {\rm C}(23) & -179.90(19) \\ {\rm R}(1) - {\rm N}(1) - {\rm C}(8) - {\rm C}(1) & -2.0(3) & {\rm N}(3) - {\rm C}(1) - {\rm C}(24)$ | Cl(1)-Ru(1)-N(1)-C(8) | 5 35(15) | C(16)-N(2)-C(18)-C(17) | 134(2) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | $R_{1}(1)-O(1)-C(1)-C(2)$ | -177 19(14) | C(10) - C(10) - C(17) C(28) - N(2) - C(18) - C(17) | -167.92(19) |
| $\begin{array}{ccccc} (1) - (2) - (2) - (2) & (1) - (2) - (2) - (2) & (1) - (2) - (2) & (1) - (2) - (2) & (1) - (2) - (2) & (1) - (2) - (2) & (1) - (2) - (2) & (1) - (2) - (2) & (1) - (2) - (2) & (1) - (2) - (2) & (2) & (2) - (2) - (2) & (2) & (2) - (2) - (2) & (2) & (2) - (2) - (2) & (2) & (2) - (2) - (2) & (2) & (2) - (2) - (2) & (2) & (2) - (2) - (2) & (2) - (2) - (2) & (2) - (2) - (2) - (2) & (2) - ($ | Ru(1)-O(1)-C(1)-C(2) | 22(3) | N(3)-C(17)-C(18)-N(2) | -107.92(19) |
| $\begin{array}{c} C(1) - C(1) - C(2) - C(3) & -1.0 + C(1) + C(1) + C(2) & -1.1 + 1.0 + C(1) + C(2) & -1.1 + 1.0 + C(1) + C(2) & -1.0 + C(2) & -1.0 + C(2) & -1.0 + C(2) & -1.0 + C(2) + C(2)$ | O(1)-C(1)-C(2)-C(3) | 1769(2) | C(16)-N(3)-C(19)-C(20) | -14.2(2) |
| $\begin{array}{c} C(1)-C(2)-C(3)-C(4)-C(5) & -2(2) & C(1)-P(1)-C(2) & 72.1(3) \\ C(2)-C(3)-C(4)-C(5) & 1.3(3) & C(1)-N(3)-C(1)-C(24) & 72.1(3) \\ C(2)-C(3)-C(4)-C(5)-C(6) & -1.8(3) & C(2)-C(1)-C(2)-C(21) & -1.8(3) \\ C(4)-C(5)-C(6)-C(7) & -179.7(2) & N(3)-C(1)-C(2)-C(25) & 179.8(2) \\ C(4)-C(5)-C(6)-C(1) & 0.1(3) & C(2)-C(2)-C(25) & 2.4(3) \\ C(2)-C(1)-C(6)-C(5) & 2.0(3) & C(1)-C(2)-C(2)-C(22) & -0.6(3) \\ O(1)-C(1)-C(6)-C(7) & 2.5(3) & C(2)-C(2)-C(2)-C(22) & -0.6(3) \\ O(1)-C(1)-C(6)-C(7) & 2.5(3) & C(2)-C(2)-C(2)-C(22) & -1.78(2) \\ C(2)-C(1)-C(6)-C(7) & -178.2(2) & C(2)-C(2)-C(2)-C(22) & -2.1(3) \\ C(2)-C(1)-C(6)-C(7) & -178.5(2) & C(2)-C(2)-C(2)-C(24) & -1.7(3) \\ C(3)-N(1)-C(7)-C(6) & -176.5(2) & C(2)-C(2)-C(2)-C(24) & -1.7(5,6(2) \\ Ru(1)-N(1)-C(7)-C(6) & -3.3(3) & C(2)-C(2)-C(2)-C(24) & -1.7(5,6(2) \\ Ru(1)-N(1)-C(7)-N(1) & -1.7(4) & C(2)-C(2)-C(2)-C(24) & -1.7(5,6(2) \\ C(1)-C(6)-C(7)-N(1) & -1.7(4) & C(2)-C(2)-C(2)-C(24) & -1.7(5,6(2) \\ C(1)-C(6)-C(7)-N(1) & -1.7(4) & C(2)-C(2)-C(2)-C(2) & -2.7(3) \\ C(7)-N(1)-C(8)-C(1) & 9.2.8(2) & C(2)-C(1)-C(24)-C(27) & -178.3(2) \\ C(1)-C(8)-C(9)-C(10) & -2.0(3) & N(3)-C(1)-C(24)-C(23) & -179.90(19) \\ Ru(1)-N(1)-C(8)-C(1) & -2.0(3) & N(3)-C(1)-C(24)-C(23) & -179.90(19) \\ Ru(1)-N(1)-C(8)-C(10) & -2.0(3) & N(3)-C(1)-C(24)-C(23) & -179.90(19) \\ C(13)-C(8)-C(9)-C(10) & 176.53(19) & C(16)-N(2)-C(28)-C(33) & -95.2(3) \\ C(13)-C(8)-C(9)-C(10) & 176.53(19) & C(16)-N(2)-C(28)-C(33) & -95.2(3) \\ C(13)-C(8)-C(9)-C(10) & 176.53(19) & C(16)-N(2)-C(28)-C(33) & -95.2(3) \\ C(13)-C(8)-C(9)-C(10) & 176.53(19) & C(16)-N(2)-C(28)-C(29) & -90.2(3) \\ C(8)-C(9)-C(10)-C(11) & -178.7(2) & C(38)-C(28)-C(29) & -90.2(3) \\ C(13)-C(8)-C(9)-C(11) & -178.7(2) & C(39)-C(39)-C(31) & -0.6(3) \\ C(13)-C(10)-C(11)-C(12) & 1.4(3) & N(2)-C(28)-C(29)-C(34) & 2.2(3) \\ R(1)-C(1)-C(12)-C(13) & 178.16(16) & C(28)-C(29)-C(30) & -2.9(3) \\ C(10)-C(11)-C(12)-C(13) & 178.5(2) & C(3)-C(3)-C(31) & -173.5(19) \\ C(10)-C(11)-C(12)-C(13) & 178.6(2) & C(3)-C(3)-C(31) & -173.6(2) \\ C(10)-C(11)-C(12)-C(13) & 177.3(2) & C(29)-C(30)-C(31) & -0.5(3)$ | C(6)-C(1)-C(2)-C(3) | -2 5(3) | C(17)-N(3)-C(19)-C(20) | 81 6(3) |
| $\begin{array}{c} C(1)-C(2)-C(2)-C(2)-C(2) & 0.53(7) & C(1))-C(1)-C(24) &$ | C(1)-C(2)-C(3)-C(4) | -2.5(5) | C(16)-N(3)-C(19)-C(20) | 72 1(3) |
| $\begin{array}{c} C(2) C(4) C(5) C(6) & 1.5.(3) & C(1) P(C) C(2) C(2) & 1.5.(3) \\ C(4) C(5) C(6) - C(7) & -179.7(2) & N(3) C(19) - C(20) - C(2) & 1.79.28(19) \\ C(4) - C(5) - C(6) - C(1) & 0.1(3) & C(24) - C(19) - C(20) - C(2) & 2.4(3) \\ C(2) - C(1) - C(6) - C(5) & 2.0(3) & C(19) - C(20) - C(2) & 2.2(3) \\ C(2) - C(1) - C(6) - C(7) & 2.5(3) & C(25) - C(20) - C(2) - C(22) & 4.6(3) \\ O(1) - C(1) - C(6) - C(7) & 2.5(3) & C(25) - C(20) - C(2) - C(22) & 2.6(3) \\ C(2) - C(1) - C(6) - C(7) & 2.5(3) & C(25) - C(20) - C(2) - C(22) & 4.6(3) \\ O(1) - C(1) - C(6) - C(7) & -178.2(2) & C(20) - C(21) - C(22) - C(23) & 2.1(3) \\ C(2) - C(1) - C(6) - C(7) & -178.2(2) & C(20) - C(21) - C(22) - C(23) & -176.6(2) \\ N(1) - N(1) - C(7) - C(6) & -176.5(2) & C(20) - C(21) - C(22) - C(23) - C(24) & -1.2(3) \\ C(5) - C(6) - C(7) - N(1) & 1.78.1(2) & C(26) - C(22) - C(23) - C(24) & -1.2(3) \\ C(5) - C(6) - C(7) - N(1) & -1.7.(4) & C(22) - C(23) - C(24) - C(27) & -178.8(2) \\ N(1) - N(1) - C(8) - C(19) & 92.9(2) & C(20) - C(19) - C(24) - C(23) & 2.7(3) \\ C(7) - N(1) - C(8) - C(13) & 84.8(2) & N(3) - C(19) - C(24) - C(23) & -179.90(19) \\ N(1) - N(1) - C(8) - C(13) & -88.5(2) & C(20) - C(19) - C(24) - C(23) & -179.90(19) \\ N(1) - N(1) - C(8) - C(13) & -88.5(2) & C(20) - C(19) - C(24) - C(23) & -179.90(19) \\ N(1) - C(8) - C(9) - C(10) & -2.0(3) & N(3) - C(19) - N(2) - C(28) - C(29) & -30.3(3) \\ C(13) - C(8) - C(9) - C(14) & 177.02) & C(18) - N(2) - C(28) - C(29) & -30.3(3) \\ C(13) - C(8) - C(9) - C(14) & 177.30(2) & C(16) - N(2) - C(28) - C(29) & -30.3(3) \\ C(13) - C(8) - C(9) - C(14) & -178.10(16) & C(33) - C(28) - C(29) - C(30) & -2.9(3) \\ C(10) - C(11) - C(12) - C(13) & 178.10(16) & C(33) - C(28) - C(29) - C(30) & -2.9(3) \\ C(10) - C(11) - C(12) - C(13) & 178.10(16) & C(33) - C(28) - C(29) - C(30) & -177.35(19) \\ C(9) - C(10) - C(11) - (12) - C(13) & 178.10(16) & C(23) - C(33) & -177.35(19) \\ C(10) - C(11) - C(12) - C(13) & 178.10(16) & C(23) - C(33) - C(33) & -2.9(3) \\ C(10) - C(11) - C(12) - C(13) & 177.36(2) & C(23) - C(33) & -177.35(2) \\ C(10) - C(11)$ | C(2)-C(3)-C(4)-C(5) | 13(3) | C(17)-N(3)-C(19)-C(24) | -95.9(3) |
| $\begin{array}{c} C(3)-C(4)-C(5)-C(6)-C(7) & -179.7(2) \\ C(4)-C(5)-C(6)-C(7) & -179.7(2) \\ C(4)-C(5)-C(6)-C(1) & 0.1(3) \\ C(24)-C(5)-C(25) & 179.8(2) \\ O(1)-C(1)-C(6)-C(5) & -177.4(2) \\ N(3)-C(19)-C(20)-C(25) & 2.4(3) \\ C(2)-C(1)-C(6)-C(7) & 2.5(3) \\ C(2)-C(1)-C(6)-C(7) & 2.5(3) \\ C(2)-C(1)-C(6)-C(7) & -178.2(2) \\ C(2)-C(1)-C(6)-C(7) & -178.2(2) \\ C(2)-C(1)-C(6)-C(7) & -178.2(2) \\ C(2)-C(1)-C(6)-C(7) & -178.2(2) \\ C(2)-C(2)-C(2)-C(2)-C(2) \\ C(2)-C(2)-C(2) \\ C(2)-C(2) \\ C(2) \\ C(2)-C(2) \\ C(2) \\ C(2)-C(3) \\ C(3)-C(3) \\ C(3)-C$ | C(3)-C(4)-C(5)-C(6) | -1.8(3) | C(24)-C(19)-C(20)-C(21) | -1.8(3) |
| $\begin{array}{c} (c_1)-c_1(0)-c_1(0)-c_1(1) & (-1)^{-1}(1) & $ | C(4)-C(5)-C(6)-C(7) | -1.0(3) | N(3)-C(19)-C(20)-C(21) | -1.0(3) |
| $\begin{array}{c} C(1)-C(0)-C(1)-C(1)-C(1)-C(1)-C(2)-C(2)-C(2)-C(2)-C(2)-C(2)-C(2)-C(2$ | C(4)-C(5)-C(6)-C(1) | 0.1(3) | C(24)-C(19)-C(20)-C(25) | 179.20(1)) 179.8(2) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | O(1)-C(1)-C(6)-C(5) | -177 A(2) | N(3)-C(19)-C(20)-C(25) | 2 A(3) |
| $\begin{array}{c} C(3) = C(1) - C(6) - C(7) & 2.5(3) & C(23) - C(23) - C(23) - C(23) & C(23) - C(23) \\ C(2) - C(1) - C(6) - C(7) & -178.2(2) & C(20) - C(21) - C(22) - C(23) & 2.1(3) \\ C(3) - N(1) - C(7) - C(6) & -176.5(2) & C(20) - C(21) - C(22) - C(26) & -176.6(2) \\ Ru(1) - N(1) - C(7) - C(6) & -3.3(3) & C(21) - C(22) - C(23) - C(24) & -1.2(3) \\ C(5) - C(6) - C(7) - N(1) & 178.1(2) & C(26) - C(22) - C(23) - C(24) & -1.2(3) \\ C(5) - C(6) - C(7) - N(1) & -1.7(4) & C(22) - C(23) - C(24) & -1.7(5) \\ C(7) - N(1) - C(8) - C(9) & 93.8(2) & C(22) - C(23) - C(24) - C(19) & -1.1(3) \\ C(7) - N(1) - C(8) - C(9) & 92.9(2) & C(20) - C(19) - C(24) - C(23) & -179.90(19) \\ Ru(1) - N(1) - C(8) - C(13) & 84.8(2) & N(3) - C(19) - C(24) - C(23) & -179.90(19) \\ Ru(1) - N(1) - C(8) - C(13) & -88.5(2) & C(20) - C(19) - C(24) - C(27) & -178.3(2) \\ C(13) - C(8) - C(9) - C(14) & 177.0(2) & C(16) - N(2) - C(28) - C(33) & -83.2(3) \\ N(1) - C(8) - C(9) - C(14) & 177.0(2) & C(18) - N(2) - C(28) - C(33) & -83.2(3) \\ N(1) - C(8) - C(9) - C(14) & -4.5(3) & C(16) - N(2) - C(28) - C(29) & -90.2(3) \\ C(4) - C(9) - C(10) - C(11) & 0.3(3) & C(18) - N(2) - C(28) - C(29) & -90.2(3) \\ C(4) - C(9) - C(10) - C(11) & -178.7(2) & C(33) - C(28) - C(29) - C(30) & -177.35(19) \\ C(9) - C(10) - C(11) - C(12) & 1.4(3) & N(2) - C(28) - C(29) - C(30) & -177.35(19) \\ C(9) - C(10) - C(11) - C(12) & 1.4(3) & N(2) - C(28) - C(29) - C(30) & -177.35(19) \\ C(9) - C(10) - C(11) - C(12) & 1.7(3) & C(29) - C(30) - C(31) & -179.6(2) \\ C(11) - C(12) - C(13) & -1.3(3) & N(2) - C(28) - C(29) - C(34) & 2.2(3) \\ B(1) - C(11) - C(12) - C(13) & -1.3(3) & N(2) - C(28) - C(29) - C(34) & 2.2(3) \\ B(1) - C(11) - C(12) - C(13) & -1.75.6(2) & C(30) - C(31) - C(32) - C(33) & -0.5(3) \\ C(9) - C(8) - C(13) - C(15) & 5.8(3) & C(29) - C(30) - C(31) - C(32) & -177.3(2) \\ N(1) - C(8) - C(13) - C(15) & 5.8(3) & C(29) - C(33) - C(32) & -177.3(2) \\ N(1) - C(8) - C(13) - C(15) & 5.8(3) & C(29) - C(33) - C(36) & -177.7(2) \\ C(19) - N(3) - C(16) - N(2) & -175.5(2) & C(31) - C(32) - C(33) - C(36) & -173.7(2) \\ $ | C(2)-C(1)-C(6)-C(5) | 20(3) | C(19)-C(20)-C(21)-C(22) | -0.6(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | O(1)-C(1)-C(6)-C(7) | 2.0(3) | C(25)-C(20)-C(21)-C(22) | 177 8(2) |
| $\begin{array}{c} C(2) = C(1) - C(7) - C(6) & -176.5(2) & C(20) - C(21) - C(22) - C(26) & -1.76.6(2) \\ Ru(1) - N(1) - C(7) - C(6) & -3.3(3) & C(21) - C(22) - C(23) - C(24) & -1.2(3) \\ C(5) - C(6) - C(7) - N(1) & 178.1(2) & C(26) - C(22) - C(23) - C(24) & 177.5(2) \\ C(1) - C(6) - C(7) - N(1) & -1.7(4) & C(22) - C(23) - C(24) - C(27) & 179.8(2) \\ Ru(1) - N(1) - C(8) - C(9) & -93.8(2) & C(22) - C(23) - C(24) - C(23) & -179.90(19) \\ Ru(1) - N(1) - C(8) - C(13) & 84.8(2) & N(3) - C(19) - C(24) - C(23) & -179.90(19) \\ Ru(1) - N(1) - C(8) - C(13) & -88.5(2) & C(20) - C(19) - C(24) - C(27) & -178.3(2) \\ C(13) - C(8) - C(9) - C(10) & -2.0(3) & N(3) - C(19) - C(24) - C(27) & -178.3(2) \\ C(13) - C(8) - C(9) - C(10) & 176.53(19) & C(16) - N(2) - C(28) - C(33) & -83.2(3) \\ N(1) - C(8) - C(9) - C(14) & 177.0(2) & C(18) - N(2) - C(28) - C(23) & -83.2(3) \\ N(1) - C(8) - C(9) - C(14) & -4.5(3) & C(16) - N(2) - C(28) - C(29) & -90.2(3) \\ C(8) - C(9) - C(10) - C(11) & 0.3(3) & C(18) - N(2) - C(28) - C(29) & -90.2(3) \\ C(9) - C(10) - C(11) & -178.7(2) & C(33) - C(28) - C(29) - C(30) & -2.9(3) \\ C(9) - C(10) - C(11) - (12) & 1.4(3) & N(2) - C(28) - C(29) - C(30) & -177.35(19) \\ C(9) - C(10) - C(11) - C(12) & 1.4(3) & N(2) - C(28) - C(29) - C(30) & -177.35(19) \\ C(9) - C(10) - C(11) - C(12) & 1.4(3) & N(2) - C(28) - C(29) - C(34) & 2.2(3) \\ Br(1) - C(11) - C(12) - C(13) & -1.3(3) & N(2) - C(28) - C(29) - C(34) & 2.2(3) \\ Br(1) - C(11) - C(12) - C(13) & -178.10(16) & C(33) - C(28) - C(29) - C(34) & 2.2(3) \\ Br(1) - C(13) - C(18) & -0.4(3) & C(34) - C(29) - C(30) - C(31) & -179.6(2) \\ C(11) - C(12) - C(13) - C(15) & -177.3(2) & C(29) - C(30) - C(31) & -179.6(2) \\ C(11) - C(12) - C(13) - C(15) & -175.6(2) & C(35) - C(31) - C(32) & -173.3(2) \\ N(1) - C(8) - C(13) - C(15) & -175.6(2) & C(35) - C(31) - C(32) - C(33) & -0.5(3) \\ C(9) - C(8) - C(13) - C(15) & -175.6(2) & C(35) - C(31) - C(32) - C(33) & -0.5(3) \\ C(11) - N(3) - C(16) - N(2) & -173.1(2) & N(2) - C(28) - C(33) - C(36) & -177.3(2) \\ N(1) - C(8) - C(13) - C(15) & -175.6(2) & C(35) - C(31) $ | C(2)-C(1)-C(6)-C(7) | -1782(2) | C(20)-C(21)-C(22) | 21(3) |
| $\begin{array}{llllllllllllllllllllllllllllllllllll$ | C(2)-C(1)-C(0)-C(7) | -176.5(2) | C(20)-C(21)-C(22)-C(25) | -176.6(2) |
| $\begin{array}{ccccc} C(5)-C(6)-C(7)-N(1) & 178.1(2) & C(2)-C(2)-C(2) & 177.5(2) \\ C(1)-C(6)-C(7)-N(1) & -1.7(4) & C(22)-C(23)-C(24)-C(19) & -1.1(3) \\ C(7)-N(1)-C(8)-C(9) & -93.8(2) & C(22)-C(23)-C(24)-C(27) & 179.8(2) \\ Ru(1)-N(1)-C(8)-C(13) & 84.8(2) & N(3)-C(19)-C(24)-C(23) & 2.7(3) \\ C(7)-N(1)-C(8)-C(13) & 84.8(2) & N(3)-C(19)-C(24)-C(23) & -179.90(19) \\ Ru(1)-N(1)-C(8)-C(13) & -88.5(2) & C(20)-C(19)-C(24)-C(27) & -178.3(2) \\ C(13)-C(8)-C(9)-C(10) & 176.53(19) & C(16)-N(2)-C(28)-C(33) & -83.2(3) \\ N(1)-C(8)-C(9)-C(14) & 177.0(2) & C(18)-N(2)-C(28)-C(33) & -83.2(3) \\ N(1)-C(8)-C(9)-C(14) & 177.3(2) & C(18)-N(2)-C(28)-C(29) & -90.2(3) \\ C(9)-C(10)-C(11) & 0.3(3) & C(16)-N(2)-C(28)-C(29) & -90.2(3) \\ C(9)-C(10)-C(11) & -178.7(2) & C(33)-C(28)-C(29)-C(30) & -2.9(3) \\ C(9)-C(10)-C(11)-E(12) & 1.4(3) & N(2)-C(28)-C(29)-C(30) & -177.35(19) \\ C(9)-C(10)-C(11)-E(12) & 1.4(3) & N(2)-C(28)-C(29)-C(34) & 176.6(2) \\ C(10)-C(11)-C(12)-C(13) & -1.3(3) & N(2)-C(28)-C(29)-C(34) & 176.6(2) \\ C(11)-C(12)-C(13) & -1.3(3) & N(2)-C(28)-C(29)-C(34) & 1.76.6(2) \\ C(11)-C(12)-C(13) & -178.16(16) & C(28)-C(29)-C(34) & 1.77.35(19) \\ C(9)-C(10)-C(11)-C(12) & 1.73.1(2) & N(2)-C(28)-C(29)-C(33) & -1.77.3(2) \\ C(9)-C(8)-C(13)-C(15) & 177.3(2) & C(29)-C(30)-C(31)-C(35) & -1.77.3(2) \\ C(9)-C(8)-C(13)-C(15) & -175.6(2) & C(3)-C(31)-C(32) & 1.7(3) \\ C(9)-C(8)-C(13)-C(15) & -175.6(2) & C(3)-C(3)-C(3) & -185.(2) \\ N(1)-C(8)-C(13)-C(15) & -175.6(2) & C(3)-C(3)-C(3) & -175.6(2) \\ C(11)-C(12)-C(13)-C(15) & -175.6(2) & C(3)-C(3)-C(3) & -175.6(2) \\ C(11)-C(13)-C(15) & -175.6(2) & C(3)-C(3)-C(3) & -175.6(2) \\ C(11)-C(13)-C(15) & -175.6(2) & C(3)-C(3)-C(3) & -173.7(2) \\ C(9)-C(8)-C(13)-C(15) & -173.1(2) & N(2)-C(28)-C(3)-C(3) & -173.7(2) \\ C(19)-N(3)-C(16)-N(2) & -173.1(2) & N(2)-C(28)-C(3)-C(3) & -173.7(2) \\ C(19)-N(3)-C(16)-N(1) & -173.6(117) & C(3)-C(3)-C(3) & -173.7(2) \\ C(19)-N(3)-C(16)-N(1) & -173.6(117) & C(3)-C(3)-C(3)-C(36) & -173.7(2) \\ C(19)-N(3)-C(16)-N(1) & -173.6(117) & C(3)-C(3)-C(3)-C(3) & -173.6(3) \\ C(28)-N(2)-C(16)-N(3) & -6.2(3) & C(10)-C(3)$ | $R_{II}(1)-N(1)-C(7)-C(6)$ | -33(3) | C(21)-C(22)-C(23)-C(24) | -1.2(3) |
| $\begin{array}{c} C(3) \in C(3) = C(7) + C(1) \\ C(1) = C(6) = C(7) + C(1) \\ C(1) = C(8) + C(9) \\ C(1) = C(8) + C(9) \\ C(1) = C(8) + C(13) \\ C(1) = C(8) + C(13) \\ C(1) = C(13) + C(13) \\ C(1) = C(13) + C(13) \\ C(13) + C(13) + C(13) \\ C(14) + C(9) + C(14) \\ C(14) + C(9) + C(14) \\ C(14) + C(13) + C(11) \\ C(13) + C(13) + C(11) \\ C(13) + C(13) + C(11) \\ C(13) + C(13) + C(13) \\ C(14) + C(13) + C(11) \\ C(13) + C(13) + C(13) \\ C(14) + C(13) + C(13) \\ C(14) + C(13) + C(13) \\ C(14) + C(13) + C(13) \\ C(13) + C(13) \\ C(13) + C(13) + C(13) \\ C(13) + C(13) \\ C(13) + C(13) \\ C(13) + C(13)$ | C(5)-C(6)-C(7)-N(1) | 178 1(2) | C(26)-C(22)-C(23)-C(24) | 1775(2) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(1)-C(6)-C(7)-N(1) | -170.1(2) | C(22)-C(23)-C(24)-C(19) | -1 1(3) |
| $\begin{array}{c} C(1) \cap (1) - C(2) - C(2$ | C(7)-N(1)-C(8)-C(9) | -93 8(2) | C(22) - C(23) - C(24) - C(17) | 179.8(2) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | $R_{1}(1)-N(1)-C(8)-C(9)$ | 92 9(2) | C(22) - C(23) - C(24) - C(23) | 27(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(7)-N(1)-C(8)-C(13) | 84 8(2) | N(3)-C(19)-C(24)-C(23) | -179.90(19) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | $R_{\rm II}(1)$ - $N(1)$ - $C(8)$ - $C(13)$ | -88 5(2) | C(20)-C(19)-C(24)-C(27) | -1783(2) |
| $\begin{array}{c} C(1) > C(3) - C(1) > C($ | C(13)-C(8)-C(9)-C(10) | -20(3) | N(3)-C(19)-C(24)-C(27) | -0.8(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | N(1)-C(8)-C(9)-C(10) | 17653(19) | C(16)-N(2)-C(28)-C(33) | 95 2(3) |
| $\begin{array}{c} C(15) C(0) C(14) & -1.78.(2) & C(15) C(25) & -90.2(3) \\ C(16)-C(10)-C(11) & 0.3(3) & C(16)-N(2)-C(28)-C(29) & -90.2(3) \\ C(14)-C(9)-C(10)-C(11) & -178.7(2) & C(33)-C(28)-C(29)-C(30) & -2.9(3) \\ C(9)-C(10)-C(11)-C(12) & 1.4(3) & N(2)-C(28)-C(29)-C(30) & -177.35(19) \\ C(9)-C(10)-C(11)-Br(1) & -178.10(16) & C(33)-C(28)-C(29)-C(34) & 176.6(2) \\ C(10)-C(11)-C(12)-C(13) & -1.3(3) & N(2)-C(28)-C(29)-C(34) & 2.2(3) \\ Br(1)-C(11)-C(12)-C(13) & 178.16(16) & C(28)-C(29)-C(30)-C(31) & 0.0(3) \\ C(11)-C(12)-C(13) & -178.10(16) & C(28)-C(29)-C(30)-C(31) & -179.6(2) \\ C(11)-C(12)-C(13) & 178.16(16) & C(28)-C(29)-C(30)-C(31) & -179.6(2) \\ C(11)-C(12)-C(13)-C(18) & -0.4(3) & C(29)-C(30)-C(31)-C(32) & 1.7(3) \\ C(9)-C(8)-C(13)-C(12) & 2.0(3) & C(29)-C(30)-C(31)-C(32) & 1.77.3(2) \\ C(9)-C(8)-C(13)-C(12) & -176.52(19) & C(30)-C(31)-C(32) & -177.3(2) \\ N(1)-C(8)-C(13)-C(15) & -175.6(2) & C(35)-C(31)-C(32) & -0.5(3) \\ C(9)-C(8)-C(13)-C(15) & 5.8(3) & C(29)-C(28)-C(33)-C(32) & 178.5(2) \\ N(1)-C(8)-C(13)-C(15) & 5.8(3) & C(29)-C(28)-C(33)-C(32) & 178.42(19) \\ C(17)-N(3)-C(16)-N(2) & -173.1(2) & N(2)-C(28)-C(33)-C(36) & -173.7(2) \\ C(19)-N(3)-C(16)-N(1) & 17.8(3) & N(2)-C(28)-C(33)-C(36) & 0.7(3) \\ C(17)-N(3)-C(16)-Ru(1) & -173.61(17) & C(31)-C(32)-C(33)-C(36) & -2.3(3) \\ C(28)-N(2)-C(16)-N(3) & -6.2(3) & C(16)-Ru(1)-C(37)-C(38) & 95.1(2) \\ C(28)-N(2)-C(16)-Ru(1) & -13.8(3) & O(1)-Ru(1)-C(37)-C(38) & 95.1(2) \\ C(28)-N(2)-C(16)-Ru(1) & -13.8(3) & O(1)-Ru(1)-C(37)-C(38) & 10.1(2) \\ \end{array}$ | C(13)-C(8)-C(9)-C(14) | 177.0(2) | C(18)-N(2)-C(28)-C(33) | -83.2(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | N(1)-C(8)-C(9)-C(14) | -4 5(3) | C(16)-N(2)-C(28)-C(29) | -90.2(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(8)-C(9)-C(10)-C(11) | 0.3(3) | C(18)-N(2)-C(28)-C(29) | 91.3(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(14)-C(9)-C(10)-C(11) | -178.7(2) | C(33)-C(28)-C(29)-C(30) | -2.9(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(9)-C(10)-C(11)-C(12) | 1.4(3) | N(2)-C(28)-C(29)-C(30) | -177.35(19) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(9)-C(10)-C(11)-Br(1) | -178.10(16) | C(33)-C(28)-C(29)-C(34) | 176.6(2) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(10)-C(11)-C(12)-C(13) | -1.3(3) | N(2)-C(28)-C(29)-C(34) | 2.2(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | Br(1)-C(11)-C(12)-C(13) | 178.16(16) | C(28)-C(29)-C(30)-C(31) | 0.0(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(11)-C(12)-C(13)-C(8) | -0.4(3) | C(34)-C(29)-C(30)-C(31) | -179.6(2) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(11)-C(12)-C(13)-C(15) | 177.3(2) | C(29)-C(30)-C(31)-C(32) | 1.7(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(9)-C(8)-C(13)-C(12) | 2.0(3) | C(29)-C(30)-C(31)-C(35) | -177.3(2) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | N(1)-C(8)-C(13)-C(12) | -176.52(19) | C(30)-C(31)-C(32)-C(33) | -0.5(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(9)-C(8)-C(13)-C(15) | -175.6(2) | C(35)-C(31)-C(32)-C(33) | 178.5(2) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | N(1)-C(8)-C(13)-C(15) | 5.8(3) | C(29)-C(28)-C(33)-C(32) | 4.1(3) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(19)-N(3)-C(16)-N(2) | -173.1(2) | N(2)-C(28)-C(33)-C(32) | 178.42(19) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(17)-N(3)-C(16)-N(2) | -4.4(3) | C(29)-C(28)-C(33)-C(36) | -173.7(2) |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(19)-N(3)-C(16)-Ru(1) | 17.8(3) | N(2)-C(28)-C(33)-C(36) | 0.7(3) |
| C(28)-N(2)-C(16)-N(3)175.2(2)C(31)-C(32)-C(33)-C(36)175.5(2)C(18)-N(2)-C(16)-N(3)-6.2(3)C(16)-Ru(1)-C(37)-C(38)95.1(2)C(28)-N(2)-C(16)-Ru(1)-13.8(3)O(1)-Ru(1)-C(37)-C(38)10.1(2) | C(17)-N(3)-C(16)-Ru(1) | -173.61(17) | C(31)-C(32)-C(33)-C(28) | -2.3(3) |
| C(18)-N(2)-C(16)-N(3)-6.2(3)C(16)-Ru(1)-C(37)-C(38)95.1(2)C(28)-N(2)-C(16)-Ru(1)-13.8(3)O(1)-Ru(1)-C(37)-C(38)10.1(2) | C(28)-N(2)-C(16)-N(3) | 175.2(2) | C(31)-C(32)-C(33)-C(36) | 175.5(2) |
| C(28)-N(2)-C(16)-Ru(1) -13.8(3) $O(1)-Ru(1)-C(37)-C(38)$ 10.1(2) | C(18)-N(2)-C(16)-N(3) | -6.2(3) | C(16)-Ru(1)-C(37)-C(38) | 95.1(2) |
| | C(28)-N(2)-C(16)-Ru(1) | -13.8(3) | O(1)-Ru(1)-C(37)-C(38) | 10.1(2) |

| N(1)-Ru(1)-C(37)-C(38) | -81.3(2) |
|-------------------------|------------|
| Cl(1)-Ru(1)-C(37)-C(38) | -170.3(2) |
| Ru(1)-C(37)-C(38)-C(39) | -12.3(4) |
| Ru(1)-C(37)-C(38)-C(43) | 168.22(19) |
| C(43)-C(38)-C(39)-C(40) | -0.6(3) |
| C(37)-C(38)-C(39)-C(40) | 179.9(2) |
| C(38)-C(39)-C(40)-C(41) | -0.6(4) |
| C(39)-C(40)-C(41)-C(42) | 1.2(4) |
| C(40)-C(41)-C(42)-C(43) | -0.4(5) |
| C(41)-C(42)-C(43)-C(38) | -0.9(5) |
| C(39)-C(38)-C(43)-C(42) | 1.4(4) |
| C(37)-C(38)-C(43)-C(42) | -179.1(2) |
| | |

Symmetry transformations were used to generate equivalent atoms.