# Magnetostructural Studies on zigzag One-Dimensional Coordination Polymers Formed by Tetraaminatodiruthenium(II,III) Paddlewheel Units Bridged by SCN Ligands

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**Table 1.** Crystal data and structure refinement for complex **1.**

| | |
|---|---|
| Empirical formula | $C_{40}H_{48}BF_4N_4O_6Ru_2$ |
| Formula weight | 969.77 |
| Temperature/K | 293(2) |
| Crystal system | triclinic |
| Space group | *P-1* |
| *a*/Å | 10.4084(8) |
| *b*/Å | 10.9075(8) |
| *c*/Å | 11.2986(9) |
| *α*/° | 67.0540(10) |
| *β*/° | 67.4970(10) |
| *γ*/° | 71.4570(10) |
| Volume/Å$^3$ | 1069.59(14) |
| Z | 1 |
| $\rho_{calc}$ g/cm$^3$ | 1.506 |
| $\mu$/mm$^{-1}$ | 0.772 |
| F(000) | 493.0 |
| Crystal size/mm$^3$ | 0.31 × 0.23 × 0.15 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.098 to 50.006 |
| Index ranges | $-11 \le h \le 12$, $-12 \le k \le 12$, $-13 \le l \le 9$ |
| Reflections collected | 8189 |
| Independent reflections | 3667 [Rint = 0.0285, Rsigma = 0.0300] |
| Data/restraints/parameters | 3667/2/238 |
| Goodness-of-fit on F$^2$ | 1.092 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0627, $wR_2$ = 0.1934 |
| Final R indexes [all data] | $R_1$ = 0.0695, $wR_2$ = 0.2034 |
| Largest diff. peak/hole / e Å$^{-3}$ | 2.57/-1.00 |

**Table S2.** Bond Lengths for complex **1**.

| **Atoms** | **Length/Å** | **Atoms** | **Length/Å** |
|---|---|---|---|
| C(1) C(2) | 1.481(9) | C(14) C(15) | 1.352(15) |
| C(1) O(2)[1] | 1.321(8) | C(17) C(18) | 1.453(14) |
| C(1) N(1) | 1.290(8) | C(17) O(3) | 1.421(11) |
| C(2) C(3) | 1.392(10) | C(18) C(19) | 1.436(15) |
| C(2) C(7) | 1.380(10) | C(19) C(20) | 1.440(13) |
| C(3) C(4) | 1.411(11) | C(20) O(3) | 1.410(10) |
| C(3) C(8) | 1.498(13) | O(1) C(9)[1] | 1.299(8) |
| C(4) C(5) | 1.319(14) | O(1) Ru(1) | 2.033(5) |
| C(5) C(6) | 1.408(14) | O(2) C(1)[1] | 1.321(8) |
| C(6) C(7) | 1.372(11) | O(2) Ru(1) | 2.039(5) |
| C(9) C(10) | 1.496(9) | N(1) Ru(1) | 2.042(4) |
| C(9) O(1)[1] | 1.299(8) | N(2) Ru(1) | 2.042(4) |
| C(9) N(2) | 1.297(8) | O(3) Ru(1) | 2.299(4) |
| C(10) C(11) | 1.375(12) | Ru(1) Ru(1)[1] | 2.2794(8) |
| C(10) C(15) | 1.424(12) | B(1) F(1) | 1.410(5) |
| C(11) C(12) | 1.441(14) | B(1) F(1)[2] | 1.410(5) |
| C(11) C(16) | 1.434(15) | B(1) F(2)[2] | 1.434(5) |
| C(12) C(13) | 1.325(18) | B(1) F(2) | 1.434(5) |
| C(13) C(14) | 1.355(19) | | |

[1]1-X,1-Y,1-Z; [2]1-X,1-Y,-Z

**Table S3.** Bond Angles for complex **1.**

| **Atoms** | **Angle/°** | **Atoms** | **Angle/°** |
|---|---|---|---|
| O(2)1 C(1) C(2) | 120.4(6) | O(3) C(20)C(19) | 109.3(7) |
| N(1) C(1) C(2) | 119.1(5) | C(9)1 O(1) Ru(1) | 121.1(5) |
| N(1) C(1) O(2)[1] | 120.6(6) | C(1)1 O(2) Ru(1) | 121.0(5) |
| C(3) C(2) C(1) | 121.9(7) | C(1) N(1) Ru(1) | 118.7(4) |
| C(7) C(2) C(1) | 118.5(6) | C(9) N(2) Ru(1) | 118.3(4) |
| C(7) C(2) C(3) | 119.6(7) | C(17) O(3) Ru(1) | 126.9(5) |
| C(2) C(3) C(4) | 117.4(8) | C(20) O(3) C(17) | 108.8(6) |
| C(2) C(3) C(8) | 121.5(7) | C(20) O(3) Ru(1) | 123.8(5) |
| C(4) C(3) C(8) | 121.0(8) | O(1) Ru(1) O(2) | 89.0(2) |
| C(5) C(4) C(3) | 122.8(8) | O(1) Ru(1) N(1) | 90.9(2) |
| C(4) C(5) C(6) | 119.9(8) | O(1) Ru(1) N(2) | 179.32(16) |
| C(7) C(6) C(5) | 118.6(9) | O(1) Ru(1) O(3) | 92.5(2) |
| C(6) C(7) C(2) | 121.6(8) | O(1) Ru(1) Ru(1)[1] | 88.53(15) |
| O(1)1 C(9) C(10) | 120.8(6) | O(2) Ru(1) N(1) | 179.66(17) |
| N(2) C(9) C(10) | 118.0(5) | O(2) Ru(1) N(2) | 90.6(2) |
| N(2) C(9) O(1)[1] | 121.1(6) | O(2) Ru(1) O(3) | 94.1(2) |
| C(11) C(10) C(9) | 120.7(7) | O(2) Ru(1) Ru(1)[1] | 88.39(15) |
| C(11) C(10) C(15) | 121.2(8) | N(1) Ru(1) N(2) | 89.57(18) |
| C(15) C(10) C(9) | 118.1(8) | N(1) Ru(1) O(3) | 86.20(18) |
| C(10) C(11) C(12) | 115.8(10) | N(1) Ru(1) Ru(1)[1] | 91.29(12) |
| C(10) C(11) C(16) | 121.1(8) | N(2) Ru(1) O(3) | 88.00(17) |
| C(16) C(11) C(12) | 123.1(10) | N(2) Ru(1) Ru(1)[1] | 90.94(12) |
| C(13) C(12) C(11) | 120.9(12) | Ru(1)1 Ru(1) O(3) | 177.28(13) |
| C(12) C(13) C(14) | 123.2(12) | F(1) B(1) F(1)[2] | 180.0 |
| C(15) C(14) C(13) | 119.1(12) | F(1) B(1) F(2) | 81.6(7) |
| C(14) C(15) C(10) | 119.8(12) | F(1)2 B(1) F(2)[2] | 81.6(7) |
| O(3) C(17) C(18) | 106.8(8) | F(1) B(1) F(2)[2] | 98.4(7) |
| C(19) C(18) C(17) | 108.5(9) | F(1)2 B(1) F(2) | 98.4(7) |
| C(18) C(19) C(20) | 105.9(9) | F(2)2 B(1) F(2) | 180.0 |

[1]1-X,1-Y,1-Z; [2]1-X,1-Y,-Z

**Table S4**. Crystal data and structure refinement for complex **2**

| | |
|---|---|
| Empirical formula | $C_{33}H_{32}N_5O_4Ru_2S$ |
| Formula weight | 796.83 |
| Temperature/K 2 | 96.15 |
| Crystal system | triclinic |
| Space group | *P-1* |
| *a*/Å | 11.4616(15) |
| *b*/Å | 11.6233(15) |
| *c*/Å | 14.6351(19) |
| *α*/° | 99.536(2) |
| *β*/° | 106.323(2) |
| *γ*/° | 106.346(2) |
| Volume/Å$^3$ | 1730.9(4) |
| Z | 2 |
| *ρ* calc g/cm$^3$ | 1.529 |
| μ/mm$^{-1}$ | 0.975 |
| F(000) | 802.0 |
| Crystal size/mm$^3$ | 0.12 × 0.11 × 0.07 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 3.008 to 50.008 |
| Index ranges | $-11 \leq h \leq 13$, $-13 \leq k \leq 13$, $-17 \leq l \leq 17$ |
| Reflections collected | 13179 |
| Independent reflections | 5918 [Rint = 0.0576, Rsigma = 0.0994] |
| Data/restraints/parameters | 5918/119/322 |
| Goodness-of-fit on F2 | 1.027 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0671, $wR_2$ = 0.1607 |
| Final R indexes [all data] | $R_1$ = 0.1367, $wR_2$ = 0.2078 |
| Largest diff. peak/hole / e Å$^{-3}$ | 1.97/-1.33 |

**Table S5.** Bond Lengths for complex **2**

| Atoms | Length/Å | Atoms | Length/Å |
|---|---|---|---|
| C(1) C(2) | 1.496(12) | C(21) C(22) | 1.3900 |
| C(1) N(2)1 | 1.297(14) | C(22) C(23) | 1.3900 |
| C(1) O(1) | 1.285(13) | C(23) C(24) | 1.3900 |
| C(2) C(3) | 1.3900 | C(26) C(27) | 1.480(15) |
| C(2) C(7) | 1.3900 | C(26) N(3)[2] | 1.319(15) |
| C(3) C(4) | 1.3900 | C(26) O(4) | 1.280(14) |
| C(3) C(8) | 1.50(2) | C(27) C(28) | 1.3900 |
| C(4) C(5) | 1.3900 | C(27) C(32) | 1.3900 |
| C(5) C(6) | 1.3900 | C(28) C(29) | 1.3900 |
| C(6) C(7) | 1.3900 | C(28) C(33) | 1.468(17) |
| C(9) C(10) | 1.464(12) | C(29) C(30) | 1.3900 |
| C(9) N(1)[1] | 1.308(13) | C(30) C(31) | 1.3900 |
| C(9) O(2) | 1.284(12) | C(31) C(32) | 1.3900 |
| C(10)C(11) | 1.3900 | N(1) C(9)[1] | 1.307(13) |
| C(10) C(15) | 1.3900 | N(1) Ru(1) | 2.037(8) |
| C(11) C(12) | 1.3900 | N(2) C(1)[1] | 1.297(14) |
| C(11) C(16) | 1.37(2) | N(2) Ru(1) | 2.019(9) |
| C(12) C(13) | 1.3900 | N(5) Ru(2) | 2.237(10) |
| C(13) C(14) | 1.3900 | N(4) C(18)2 | 1.268(16) |
| C(14) C(15) | 1.3900 | N(4) Ru(2) | 2.042(9) |
| C(17) N(5) | 1.156(13) | N(3) C(26)2 | 1.319(15) |
| C(17) S(1) | 1.633(11) | N(3) Ru(2) | 2.022(10) |
| C(18) C(19) | 1.496(15) | O(1) Ru(1) | 2.040(8) |
| C(18) N(4)[2] | 1.268(16) | O(2) Ru(1) | 2.039(7) |
| C(18) O(3) | 1.291(16) | O(3) Ru(2) | 2.049(8) |
| C(19) C(20) | 1.3900 | O(4) Ru(2) | 2.059(9) |
| C(19) C(24) | 1.3900 | Ru(1) Ru(1)[1] | 2.3099(18) |
| C(20) C(21) | 1.3900 | Ru(1) S(1) | 2.621(3) |
| C(20) C(25) | 1.39(3) | Ru(2) Ru(2)[2] | 2.2954(18) |

[1]1-X,1-Y,1-Z; [2]-X,-Y,-Z

**Table S6.** Bond Angles for complex **2**

| Atom | Angle/° | Atom | Angle/° |
|---|---|---|---|
| N(2)1 C(1) C(2) | 121.0(11) | C(29) C(28) C(27) | 120.0 |
| O(1) C(1) C(2) | 117.8(10) | C(29) C(28) C(33) | 117.7(10) |
| O(1) C(1) N(2)[1] | 121.1(10) | C(28) C(29) C(30) | 120.0 |
| C(3) C(2) C(1) | 120.4(8) | C(29) C(30) C(31) | 120.0 |
| C(3) C(2) C(7) | 120.0 | C(32) C(31) C(30) | 120.0 |
| C(7) C(2) C(1) | 119.6(8) | C(31) C(32) C(27) | 120.0 |
| C(2) C(3) C(4) | 120.0 | C(9)1 N(1) Ru(1) | 122.8(7) |
| C(2) C(3) C(8) | 123.8(11) | C(1)1 N(2) Ru(1) | 121.5(8) |
| C(4) C(3) C(8) | 115.6(11) | C(17) N(5) Ru(2) | 169.3(10) |
| C(3) C(4) C(5) | 120.0 | C(18)2 N(4) Ru(2) | 122.0(9) |
| C(6) C(5) C(4) | 120.0 | C(26)2 N(3) Ru(2) | 121.7(8) |
| C(5) C(6) C(7) | 120.0 | C(1) O(1) Ru(1) | 119.1(7) |
| C(6) C(7) C(2) | 120.0 | C(9) O(2) Ru(1) | 117.9(7) |
| N(1)1 C(9) C(10) | 120.9(10) | C(18) O(3) Ru(2) | 118.2(8) |
| O(2) C(9) C(10) | 118.3(10) | C(26) O(4) Ru(2) | 119.4(8) |
| O(2) C(9) N(1)[1] | 120.9(10) | N(1) Ru(1) O(1) | 90.5(3) |
| C(11) C(10) C(9) | 118.0(8) | N(1) Ru(1) O(2) | 178.3(3) |
| C(11) C(10) C(15) | 120.0 | N(1) Ru(1) Ru(1)[1] | 86.5(3) |
| C(15) C(10) C(9) | 121.9(8) | N(1) Ru(1) S(1) | 95.9(3) |
| C(12) C(11) C(10) | 120.0 | N(2) Ru(1) N(1) | 90.6(4) |
| C(16) C(11) C(10) | 123.4(12) | N(2) Ru(1) O(1) | 177.9(3) |
| C(16) C(11) C(12) | 115.7(12) | N(2) Ru(1) O(2) | 90.0(3) |
| C(13) C(12) C(11) | 120.0 | N(2) Ru(1) Ru(1)[1] | 88.4(3) |
| C(12) C(13) C(14) | 120.0 | N(2) Ru(1) S(1) | 91.9(3) |
| C(15) C(14) C(13) | 120.0 | O(1) Ru(1) Ru(1)[1] | 89.9(2) |
| C(14) C(15) C(10) | 120.0 | O(1) Ru(1) S(1) | 89.8(2) |
| N(5) C(17) S(1) | 178.0(11) | O(2) Ru(1) O(1) | 88.9(3) |
| N(4)2 C(18) C(19) | 122.4(13) | O(2) Ru(1) Ru(1)[1] | 91.9(2) |
| N(4)2 C(18) O(3) | 121.5(12) | O(2) Ru(1) S(1) | 85.7(2) |
| O(3) C(18) C(19) | 116.0(13) | Ru(1)1 Ru(1) S(1) | 177.57(9) |
| C(20) C(19) C(18) | 122.2(11) | N(5) Ru(2) Ru(2)[2] | 176.6(3) |
| C(20) C(19) C(24) | 120.0 | N(4) Ru(2) N(5) | 88.9(4) |
| C(24) C(19) C(18) | 117.8(11) | N(4) Ru(2) O(3) | 177.7(4) |
| C(19) C(20) C(25) | 123.4(13) | N(4) Ru(2) O(4) | 91.9(4) |
| C(21) C(20) C(19) | 120.0 | N(4) Ru(2) Ru(2)[2] | 87.7(3) |
| C(21) C(20) C(25) | 116.6(13) | N(3) Ru(2) N(5) | 90.9(4) |
| C(20) C(21) C(22) | 120.0 | N(3) Ru(2) N(4) | 89.4(4) |
| C(23) C(22) C(21) | 120.0 | N(3) Ru(2) O(3) | 89.1(4) |
| C(24) C(23) C(22) | 120.0 | N(3) Ru(2) O(4) | 178.1(3) |
| C(23) C(24) C(19) | 120.0 | N(3) Ru(2) Ru(2)[2] | 88.6(3) |

| | | | |
|---|---|---|---|
| N(3)2 C(26) C(27) | 120.2(11) | O(3) Ru(2) N(5) | 92.8(4) |
| O(4) C(26) C(27) | 119.7(11) | O(3) Ru(2) O(4) | 89.5(4) |
| O(4) C(26) N(3)2 | 120.0(12) | O(3) Ru(2) Ru(2)[2] | 90.6(2) |
| C(28) C(27) C(26) | 122.9(8) | O(4) Ru(2) N(5) | 90.5(4) |
| C(28) C(27) C(32) | 120.0 | O(4) Ru(2) Ru(2)[2] | 90.1(2) |
| C(32) C(27) C(26) | 117.0(8) | C(17) S(1) Ru(1) | 98.9(4) |
| C(27) C(28) C(33) | 122.3(10) | | |

[1]1-X,1-Y,1-Z; [2]-X,-Y,-Z

**Table S7.** Crystal data and structure refinement for complex **3**

| | |
|---|---|
| Empirical formula | $C_{33}H_{28}N_5O_4Ru_2S$ |
| Formula weight | 792.80 |
| Temperature/K | 296.15 |
| Crystal system | triclinic |
| Space group | *P-1* |
| *a*/Å | 11.158(3) |
| *b*/Å | 12.746(3) |
| *c*/Å | 14.768(3) |
| *α*/° | 66.649(4) |
| *β*/° | 75.001(4) |
| *γ*/° | 69.244(4) |
| Volume/Å$^3$ | 1785.9(7) |
| *Z* | 2 |
| *ρ*calcg/cm$^3$ | 1.474 |
| μ/mm$^{-1}$ | 0.945 |
| F(000) | 794.0 |
| Crystal size/mm$^3$ | 0.2 × 0.11 × 0.04 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 3.032 to 57.93 |
| Index ranges | $-15 \leq h \leq 15$, $-17 \leq k \leq 17$, $-20 \leq l \leq 19$ |
| Reflections collected | 18810 |
| Independent reflections | 8502 [Rint = 0.0660, Rsigma = 0.1250] |
| Data/restraints/parameters | 8502/0/410 |
| Goodness-of-fit on F$^2$ | 1.005 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0740, $wR_2$ = 0.2101 |
| Final R indexes [all data] | $R_1$ = 0.1611, $wR_2$ = 0.2722 |
| Largest diff. peak/hole / e Å$^{-3}$ | 1.39/-1.55 |

**Table S8.** Bond Lengths for complex **3**

| Atoms | Length/Å | Atoms | Length/Å |
|---|---|---|---|
| Ru(1) Ru(1)1 | 2.3131(15) | C(22) C(40) | 1.407(15) |
| Ru(1) S(3) | 2.643(3) | C(22) C(42) | 1.407(14) |
| Ru(1) O(6) | 2.076(6) | C(22) C(9) | 1.504(13) |
| Ru(1) O(1)[1] | 2.039(7) | C(23) C(33) | 1.390(15) |
| Ru(1) N(5) | 2.031(7) | C(26) C(45) | 1.440(15) |
| Ru(1) N(6)1 | 2.055(7) | C(27) C(31) | 1.405(15) |
| Ru(2) Ru(2)[2] | .2956(15) | C(29) C(31) | 1.369(17) |
| Ru(2) O(7) | 2.042(7) | C(29) C(41) | 1.360(18) |
| Ru(2) N(12) | 2.253(8) | C(31) C(62) | 1.493(17) |
| Ru(2) O(2) | 2.045(6) | C(33) C(36) | 1.372(17) |
| Ru(2) N(3)2 | 2.038(7) | C(33) C(50) | 1.543(17) |
| Ru(2) N(1)2 | 2.048(7) | C(35) C(47) | 1.388(17) |
| S(3) C(16) | 1.640(10) | C(35) C(51) | 1.40(2) |
| O(6) C(15) | 1.295(11) | C(36) C(12) | 1.39(2) |
| O(7) C(14) | 1.310(11) | C(38) C(41) | 1.379(15) |
| N(12) C(16) | 1.145(11) | C(39) C(12) | 1.338(17) |
| C(14) C(20) | 1.488(14) | C(40) C(55) | 1.404(17) |
| C(14) N(3) | 1.286(12) | C(42) C(46) | 1.388(15) |
| C(15) C(21) | 1.490(13) | C(45) C(51) | 1.368(18) |
| C(15) N(6) | 1.292(12) | C(45) C(13) | 1.423(19) |
| C(17) C(18) | 1.500(13) | C(46) C(49) | 1.371(19) |
| C(17) O(1) | 1.298(11) | C(46) C(0AA) | 1.486(18) |
| C(17) N(5) | 1.279(11) | C(49) C(55) | 1.367(19) |
| C(18) C(26) | 1.345(15) | O(1) Ru(1)[1] | 2.039(7) |
| C(18) C(47) | 1.415(16) | O(2) C(9) | 1.321(12) |
| C(20) C(23) | 1.387(14) | N(3) Ru(2)[2] | 2.038(7) |
| C(20) C(39) | 1.386(14) | N(6) Ru(1)[1] | 2.055(7) |
| C(21) C(27) | 1.379(14) | C(9) N(1) | 1.265(12) |
| C(21) C(38) | 1.373(14) | N(1) Ru(2)[2] | 2.048(7) |

[1]1-X,1-Y,1-Z; [2]2-X,1-Y,-Z

**Table S9.** Bond Angles for complex **3**

| **Atom**s | **Angle/**° | **Atoms** | **Angle/**° |
|---|---|---|---|
| Ru(1)$^{1}$ Ru(1) S(3) | 175.80(9) | C(23) C(20) C(14) | 120.3(9) |
| O(6) Ru(1) Ru(1)1 | 90.81(19) | C(39) C(20) C(14) | 120.8(10) |
| O(6) Ru(1) S(3) | 92.6(2) | C(39) C(20) C(23) | 118.8(10) |
| O(1)$^{1}$ Ru(1) Ru(1)$^{1}$ | 90.1(2) | C(27) C(21) C(15) | 119.0(9) |
| O(1)$^{1}$ Ru(1) S(3) | 87.6(2) | C(38) C(21) C(15) | 121.2(9) |
| O(1)$^{1}$ Ru(1) O(6) | 87.8(3) | C(38) C(21) C(27) | 119.8(10) |
| O(1)$^{1}$ Ru(1) N(6)$^{1}$ | 91.7(3) | C(40) C(22) C(9) | 120.3(10) |
| N(5) Ru(1) Ru(1)$^{1}$ | 88.1(2) | C(42) C(22) C(40) | 118.2(10) |
| N(5) Ru(1) S(3) | 94.1(2) | C(42) C(22) C(9) | 121.5(9) |
| N(5) Ru(1) O(6) | 92.9(3) | C(20) C(23) C(33) | 120.5(11) |
| N(5) Ru(1) O(1)$^{1}$ | 178.0(3) | C(18) C(26) C(45) | 121.1(11) |
| N(5) Ru(1) N(6)$^{1}$ | 87.5(3) | C(21) C(27) C(31) | 120.2(11) |
| N(6)$^{1}$ Ru(1) Ru(1)$^{1}$ | 87.8(2) | C(41) C(29) C(31) | 119.5(12) |
| N(6)$^{1}$ Ru(1) S(3) | 88.8(2) | C(27) C(31) C(62) | 118.3(12) |
| N(6)$^{1}$ Ru(1) O(6) | 178.5(3) | C(29) C(31) C(27) | 119.3(12) |
| O(7) Ru(2) Ru(2)2 | 88.0(2) | C(29) C(31) C(62) | 122.3(12) |
| O(7) Ru(2) N(12) | 90.5(3) | C(23) C(33) C(50) | 119.5(12) |
| O(7) Ru(2) O(2) | 89.8(3) | C(36) C(33) C(23) | 118.2(12) |
| O(7) Ru(2) N(1)$^{2}$ | 91.1(3) | C(36) C(33) C(50) | 122.3(13) |
| N(12) Ru(2) Ru(2)$^{2}$ | 175.9(2) | C(47) C(35) C(51) | 119.4(13) |
| O(2) Ru(2) Ru(2)$^{2}$ | 91.5(2) | C(33) C(36) C(12) | 121.4(13) |
| O(2) Ru(2) N(12) | 92.3(3) | C(21) C(38) C(41) | 119.0(12) |
| O(2) Ru(2) N(1)$^{2}$ | 178.9(3) | C(12) C(39) C(20) | 121.4(12) |
| N(3)$^{2}$ Ru(2) Ru(2)$^{2}$ | 90.60(19) | C(55) C(40) C(22) | 119.2(13) |
| N(3)$^{2}$ Ru(2) O(7) | 178.4(3) | C(29) C(41) C(38) | 122.1(12) |
| N(3)$^{2}$ Ru(2) N(12) | 90.9(3) | C(46) C(42) C(22) | 121.8(12) |
| N(3)$^{2}$ Ru(2) O(2) | 89.4(3) | C(51) C(45) C(26) | 117.0(12) |
| N(3)$^{2}$ Ru(2) N(1)$^{2}$ | 89.7(3) | C(51) C(45) C(13) | 122.6(14) |
| N(1)$^{2}$ Ru(2) Ru(2)$^{2}$ | 87.7(2) | C(13) C(45) C(26) | 120.2(14) |
| N(1)$^{2}$ Ru(2) N(12) | 88.5(3) | C(42) C(46) C(0AA) | 120.2(14) |
| C(16) S(3) Ru(1) | 98.0(3) | C(49) C(46) C(42) | 118.2(13) |
| C(15) O(6) Ru(1) | 117.4(6) | C(49) C(46) C(0AA) | 121.6(12) |
| C(14) O(7) Ru(2) | 121.7(6) | C(35) C(47) C(18) | 118.7(12) |
| C(16) N(12) Ru(2) | 159.3(8) | C(55) C(49) C(46) | 122.4(12) |
| O(7) C(14) C(20) | 120.7(9) | C(45) C(51) C(35) | 122.6(12) |
| N(3) C(14) O(7) | 119.8(9) | C(49) C(55) C(40) | 120.2(13) |
| N(3) C(14) C(20) | 119.4(9) | C(17) O(1) Ru(1)$^{1}$ | 118.5(6) |
| O(6) C(15) C(21) | 118.4(8) | C(9) O(2) Ru(2) | 116.5(6) |
| N(6) C(15) O(6) | 122.1(9) | C(14) N(3) Ru(2)$^{2}$ | 119.9(6) |
| N(6) C(15) C(21) | 119.6(8) | C(17) N(5) Ru(1) | 121.4(6) |

| | | | |
|---|---|---|---|
| N(12) C(16) S(3) | 178.3(10) | C(15) N(6) Ru(1)[1] | 121.6(6) |
| O(1) C(17) C(18) | 116.4(8) | O(2) C(9) C(22) | 115.1(9) |
| N(5) C(17) C(18) | 122.0(8) | N(1) C(9) C(22) | 122.2(9) |
| N(5) C(17) O(1) | 121.5(9) | N(1) C(9) O(2) | 122.6(8) |
| C(26) C(18) C(17) | 120.8(10) | C(39) C(12) C(36) | 119.5(13) |
| C(26) C(18) C(47) | 121.2(10) | C(9) N(1) Ru(2)[2] | 121.6(6) |
| C(47) C(18) C(17) | 117.9(10) | | |

[1]1-X,1-Y,1-Z; [2]2-X,1-Y,-Z

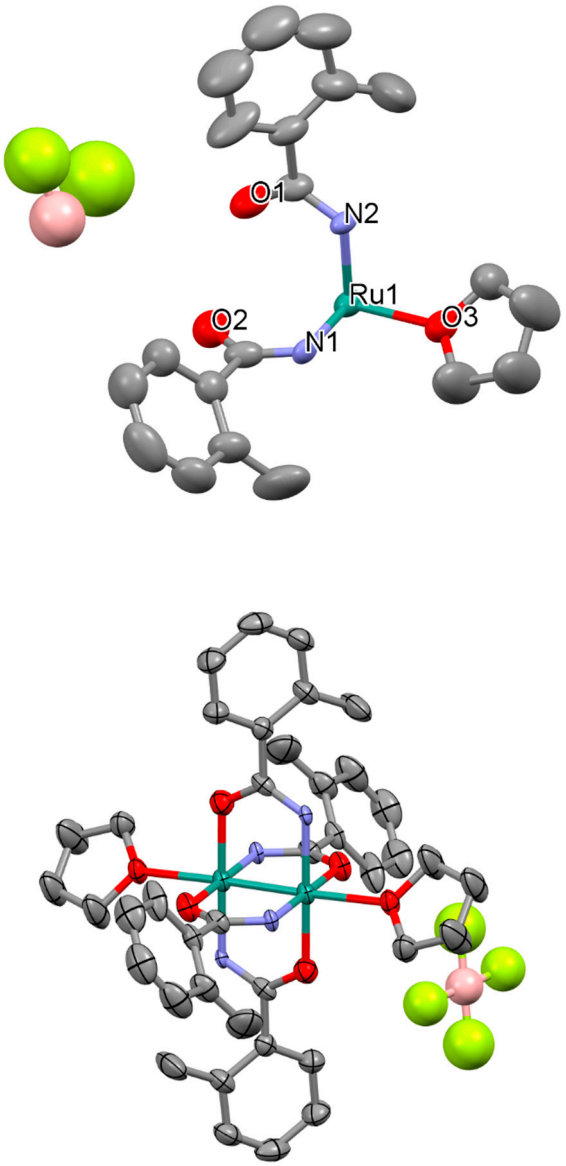


**Figure S1.** Representation showing the asymetric unit (top) and the dimetallic unit (bottom) of **1**.

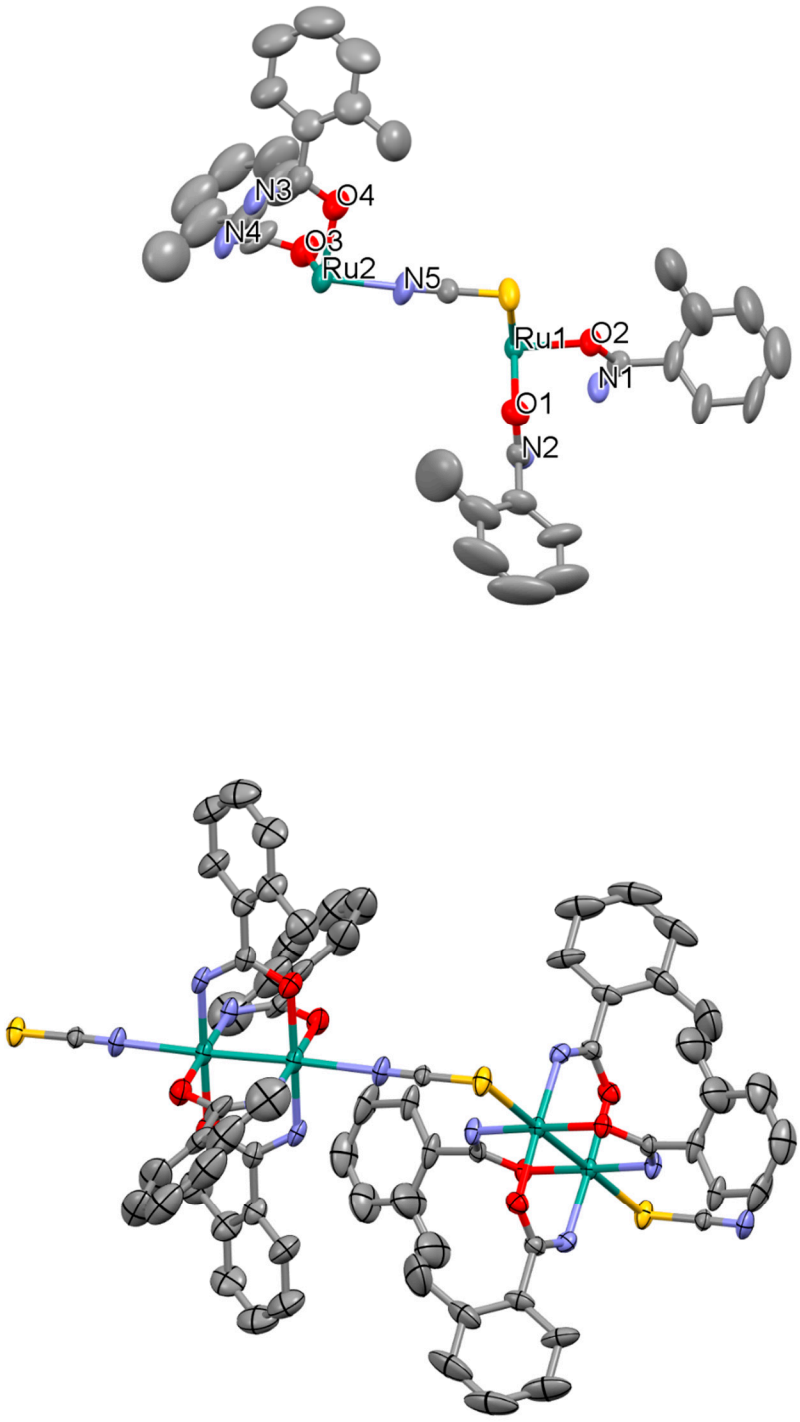


**Figure S2.** Representation of the asymetric unit (top) and the dimetallic units (bottom) that form **2**.

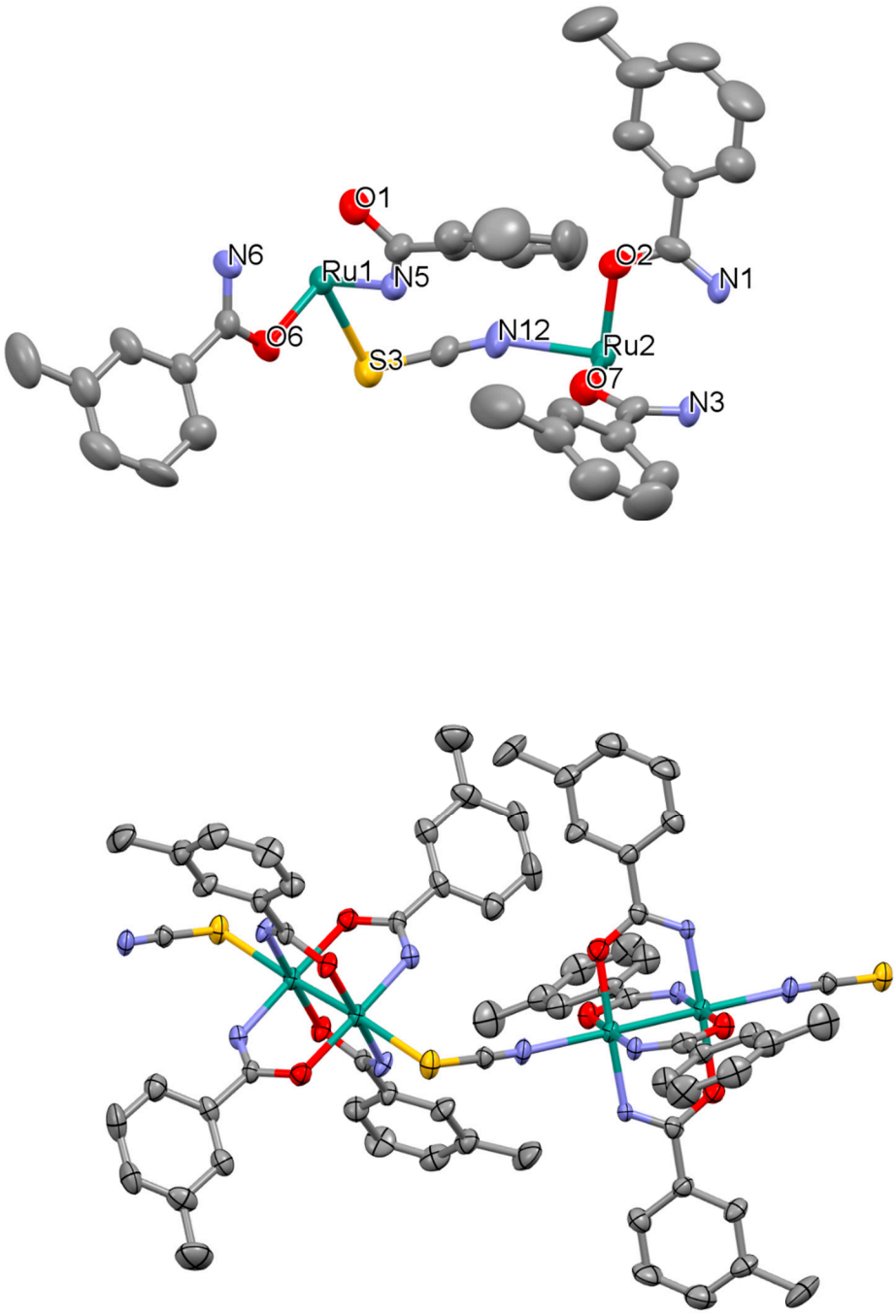


**Figure S3.** Representation of the asymetric unit (top) and the dimetallic units (bottom) that form **3**.

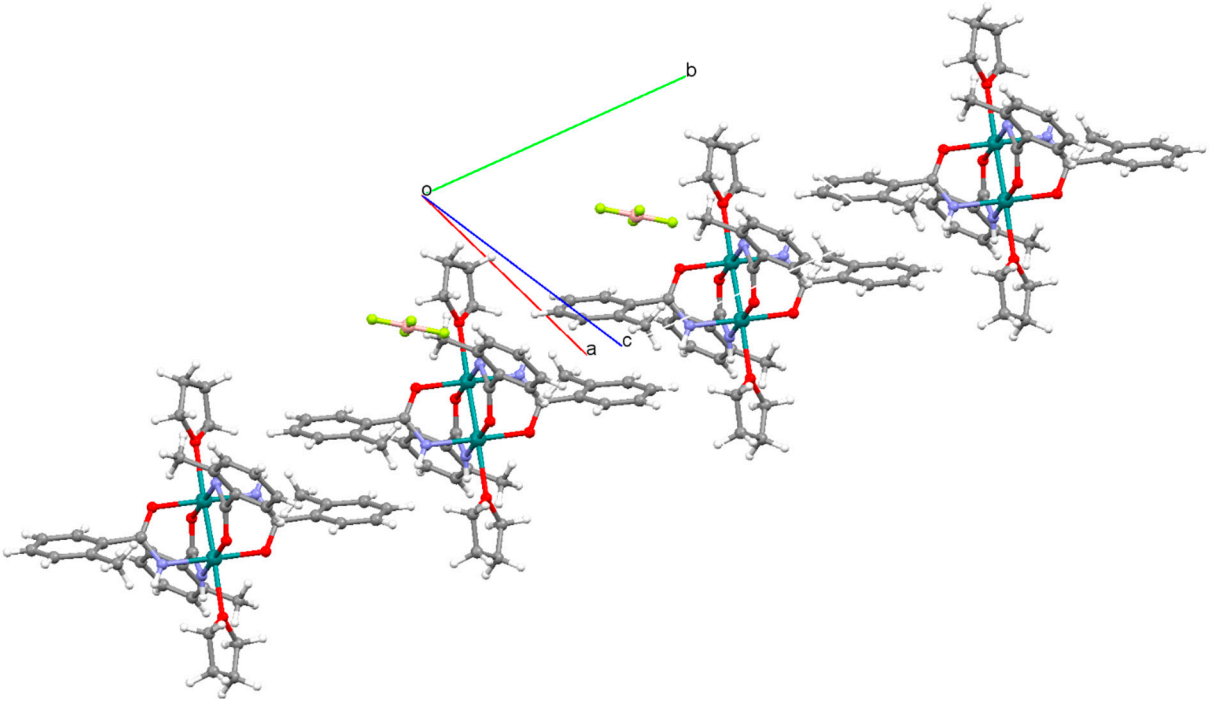


**Figure S4.** Representation of the π-π stacking observed in the structure of complex **1**.

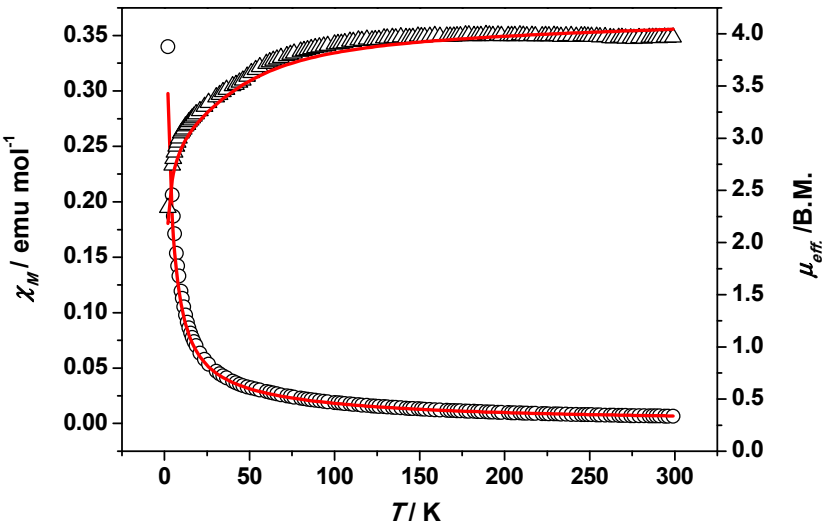


**Figure S5**. Magnetic molar susceptibility (circles) and magnetic moment (triangles) *vs.* temperature for compound **2**. Solid lines represent the best fit obtained using the model explained in the text.

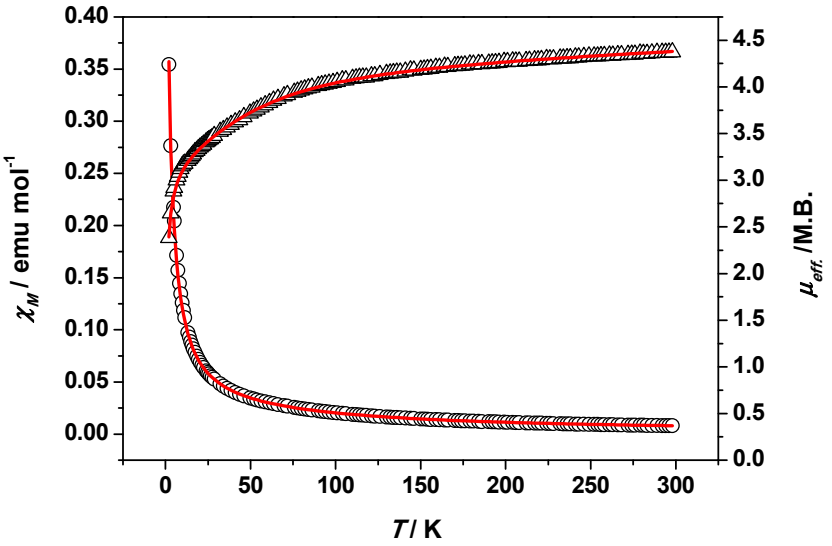


**Figure S6**. Magnetic molar susceptibility (circles) and magnetic moment (triangles) *vs.* temperature for compound **3**. Solid lines represent the best fit obtained using the model explained in the text.