

Electronic Supplementary Information for

The one pot synthesis of heterobimetallic complexes from a homoditopic pyrimidine-hydrazone
ligand

Daniel J. Hutchinson, Lyall R. Hanton, and Stephen C. Moratti*

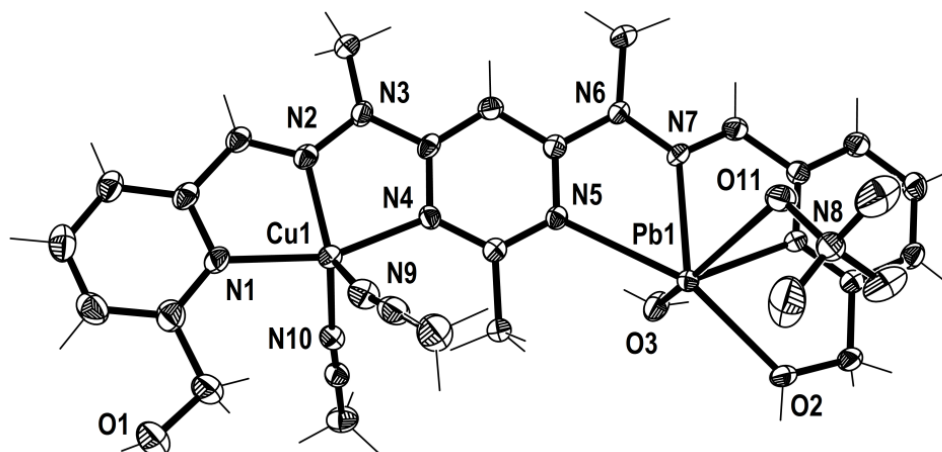
Department of Chemistry, University of Otago, PO Box 56, Dunedin, New Zealand,

*E-mail: lhanton@chemistry.otago.ac.nz

Figures S1-S3. Thermal ellipsoid views of complexes **1-3**.

Tables S1-S3. Selected bond lengths (Å) and angles (°) of complexes **1-3**.

Discussion of Disorder. Complexes **2** and **3** contained SO_3CF_3^- anions which were disordered over two sites. The site occupancy factors for the major components of the disordered anions in complexes **2** and **3** were 0.50, and 0.80, respectively.



Figures S1. View of the $[\text{CuPbL1}(\text{ClO}_4)(\text{CH}_3\text{CN})_2(\text{H}_2\text{O})]^{3+}$ cation of complex **1** (crystallographic numbering). Thermal ellipsoids are drawn at the 50 % probability level.

Table S1. Selected bond lengths (Å) and angles (°) of $[\text{CuPbL1}(\text{ClO}_4)(\text{CH}_3\text{CN})_2(\text{H}_2\text{O})](\text{ClO}_4)_3$ (**1**).

| | | | | | |
|---------|----------|-----------|----------|------------|------------|
| Cu1-N1 | 2.053(5) | Pb1-N8 | 2.507(5) | N2-Cu1-N10 | 124.9(2) |
| Cu1-N2 | 1.952(5) | Pb1-O2 | 2.552(4) | N9-Cu1-N10 | 110.9(2) |
| Cu1-N4 | 2.009(5) | Pb1-O11 | 2.710(4) | N5-Pb1-N7 | 59.70(19) |
| Cu1-N9 | 2.027(5) | Pb1-O3 | 2.411(4) | N7-Pb1-N8 | 65.52(15) |
| Cu1-N10 | 2.063(6) | N1-Cu1-N2 | 80.1(2) | N8-Pb1-O2 | 62.66(14) |
| Pb1-N5 | 2.709(5) | N2-Cu1-N4 | 79.6(2) | O2-Pb1-N5 | 152.76(15) |
| Pb1-N7 | 2.563(5) | N1-Cu1-N4 | 159.7(2) | O11-Pb1-O3 | 145.04(16) |

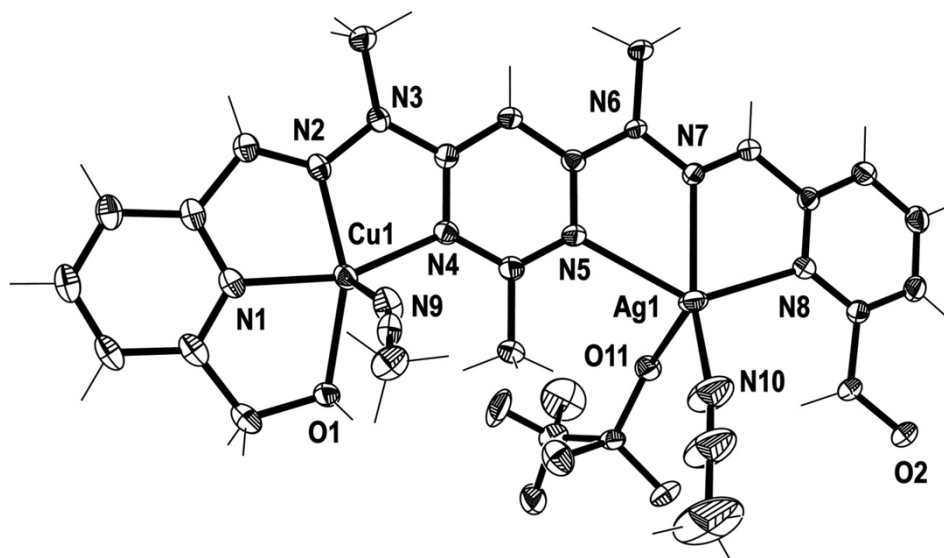


Figure S2. View of the $[\text{CuAgL1}(\text{SO}_3\text{CF}_3)(\text{CH}_3\text{CN})_2]^{2+}$ cation of complex **2** (crystallographic numbering). Thermal ellipsoids are drawn at the 50 % probability level.

Table S2. Selected bond lengths (Å) and angles (°) of $[\text{CuAgL1}(\text{SO}_3\text{CF}_3)(\text{CH}_3\text{CN})_2](\text{SO}_3\text{CF}_3)_2 \cdot \text{CH}_3\text{CN}$ (**2**).

| | | | | | |
|--------|------------|-----------|-----------|-------------|------------|
| Cu1-N1 | 1.935(2) | Ag1-N8 | 2.398(2) | N1-Cu1-N4 | 158.15(9) |
| Cu1-N2 | 1.964(2) | Ag1-N10 | 2.197(3) | N2-Cu1-O1 | 157.56(8) |
| Cu1-N4 | 1.988(2) | Ag1-O11 | 2.593(7) | N5-Ag1-N7 | 64.90(7) |
| Cu1-N9 | 2.229(2) | N1-Cu1-N2 | 80.03(9) | N7-Ag1-N8 | 69.55(7) |
| Cu1-O1 | 2.0964(19) | N2-Cu1-N4 | 79.34(8) | N7-Ag1-N10 | 148.89(11) |
| Ag1-N5 | 2.480(2) | N4-Cu1-O1 | 120.13(8) | N5-Ag1-N8 | 134.15(7) |
| Ag1-N7 | 2.391(2) | N1-Cu1-N9 | 97.04(8) | N10-Ag1-O11 | 101.51(17) |

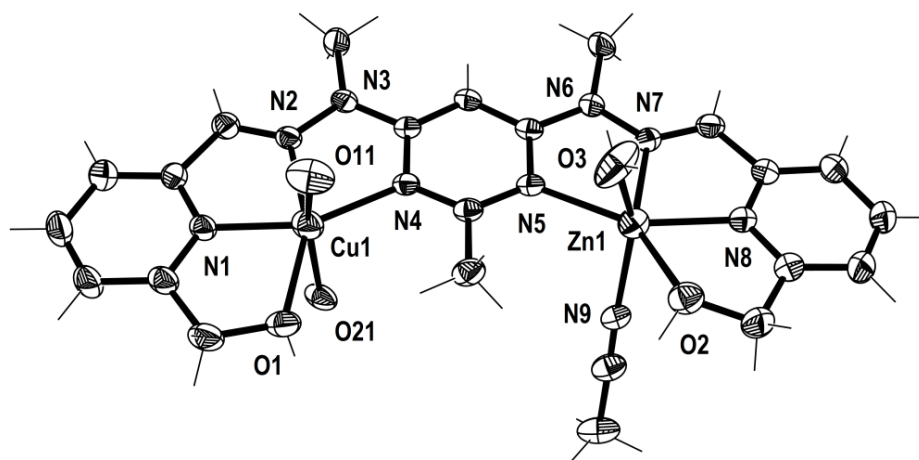


Figure S3. View of the $[\text{CuZnL1}(\text{SO}_3\text{CF}_3)_2(\text{CH}_3\text{CN})(\text{H}_2\text{O})]^{2+}$ cation of complex **3** (crystallographic numbering). Thermal ellipsoids are drawn at the 50 % probability level (the SO_3CF_3^- anions coordinated to Cu1 have been simplified to O11 and O21 for clarity).

Table S3. Selected bond lengths (Å) and angles (°) of $\text{CuZnL1}(\text{SO}_3\text{CF}_3)_2(\text{CH}_3\text{CN})(\text{H}_2\text{O})[(\text{SO}_3\text{CF}_3)_2 \cdot \text{CH}_3\text{CN}]$ (**3**).

| | | | | | |
|---------|----------|-----------|-----------|-------------|------------|
| Cu1-N1 | 1.967(3) | Zn1-N7 | 2.126(3) | N4-Cu1-O1 | 125.11(13) |
| Cu1-N2 | 2.032(3) | Zn1-N8 | 2.058(3) | O11-Cu1-O21 | 161.71(13) |
| Cu1-N4 | 2.028(3) | Zn1-N9 | 2.098(3) | N5-Zn1-N7 | 73.36(12) |
| Cu1-O1 | 2.102(3) | Zn1-O2 | 2.237(3) | N7-Zn1-N8 | 75.78(13) |
| Cu1-O11 | 2.257(3) | Zn1-O3 | 2.063(4) | N8-Zn1-O2 | 72.64(13) |
| Cu1-O21 | 2.269(3) | N1-Cu1-N2 | 78.60(13) | O2-Zn1-N5 | 138.10(12) |
| Zn1-N5 | 2.140(3) | N2-Cu1-N4 | 77.94(12) | N9-Zn1-O3 | 145.70(19) |