Supplementary Material

Magnetic and Electronic Properties of Three New Hetero-bimetallic Coordination Frameworks, [Ru$_2$(O$_2$CR)$_4$][Au(CN)$_2$] (R = benzoic acid, furan-2-carboxylate or thiophene-2-carboxylate)

Michael J. Murphy,$^A$ Tony D. Keene,$^B$ Jason R. Price,$^A$ Deanna M. D’Alessandro$^{A,C}$ and Cameron J. Kepert$^{A,C}$

$^A$ School of Chemistry, The University of Sydney, NSW, 2006, Australia.
$^B$ Chemistry, University of Southampton, Highfield, Southampton, SO17 1BJ, UK.
$^C$ Corresponding author. Email: cameron.kepert@sydney.edu.au; deanna.dalessandro@sydney.edu.au

Figure S1. Le Bail fit of the PXRD pattern for 1(Thio) at 293 K; unit cell parameters $a = 10.4064(4)$, $c = 25.8797(11)$ Å and $V = 2802.6(2)$ Å$^3$. 

Figure S2. Le Bail fit of the PXRD pattern for **1(Furan)** at 293 K; unit cell parameters
\[
a = 10.3837(3), \quad c = 25.9083(10) \ \text{Å} \quad \text{and} \quad V = 2793.50(17) \ \text{Å}^3.
\]

Figure S3. Le Bail fit of the PXRD pattern for **1(Ph)** at 293 K; unit cell parameters
\[
a = 40.296(5), \quad b = 13.5091(17), \quad c = 25.661(6) \ \text{Å}, \quad \beta = 103.521(13)^\circ \quad \text{and} \quad V = 12651(4) \ \text{Å}^3.
\]
Figure S4. a) FT–IR (red line) and Raman (black line) spectra of 1(Ph). b) Raman spectra of 1(Ph) (black), 1(Thio) (red) and 1(Furan) (blue).
Figure S5. Solid state luminescence spectrum of 1(Ph).

Figure S6. Normalised UV–Vis-NIR spectra of [Ru₂(O₂CPh)₄(THF)₂]BF₄ (black line) and 1(Ph) (red line).
**Figure S7.** UV-Vis-NIR of 1(Thio) (black line) and 1(Furan) (red line). The noise in the region 12000-12500 cm\(^{-1}\) is associated with the NIR to Vis detector changeover.
Figure S8. Plots of $\chi_M$ and $\chi_M^{-1}$ for 1(Ph). Curie–Weiss fit for $\chi^{-1}$ shown in red. Remeasurement led to a change in magnitude of the small feature at 270 K (which is present also in the data for the other compounds), indicating that it is an artefact of the measurement.

Figure S9. a) Plots of $\chi_M$ and $\chi_M^{-1}$ for 1(Thio). Curie–Weiss fit for $\chi^{-1}$ shown in red.
Figure S10. a) Plots of $\chi_M$ and $\chi_M^{-1}$ for 1(Furan). Curie–Weiss fit for $\chi^{-1}$ shown in red.

Figure S11. Thermogravimetric analysis of 1(Furan).
Figure S12. Thermogravimetric analysis of 1(Thio).

Figure S23. Thermogravimetric analysis of 1(Ph).