Supplementary Materials: Coordination of a Pyrazole Functionalized Acetylacetone to the Coinage Metal Cations: An Unexpected Packing Similarity and a Trinuclear Cu^{II}/Au^{I} Complex

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1. Powder X-Ray Diffractograms

Simulated diffraction patterns based on data collections at 100 K correspond to a smaller unit cell and therefore to larger 2θ in reciprocal space, thus resulting in a slight systematic shift between calculated and experimental patterns.

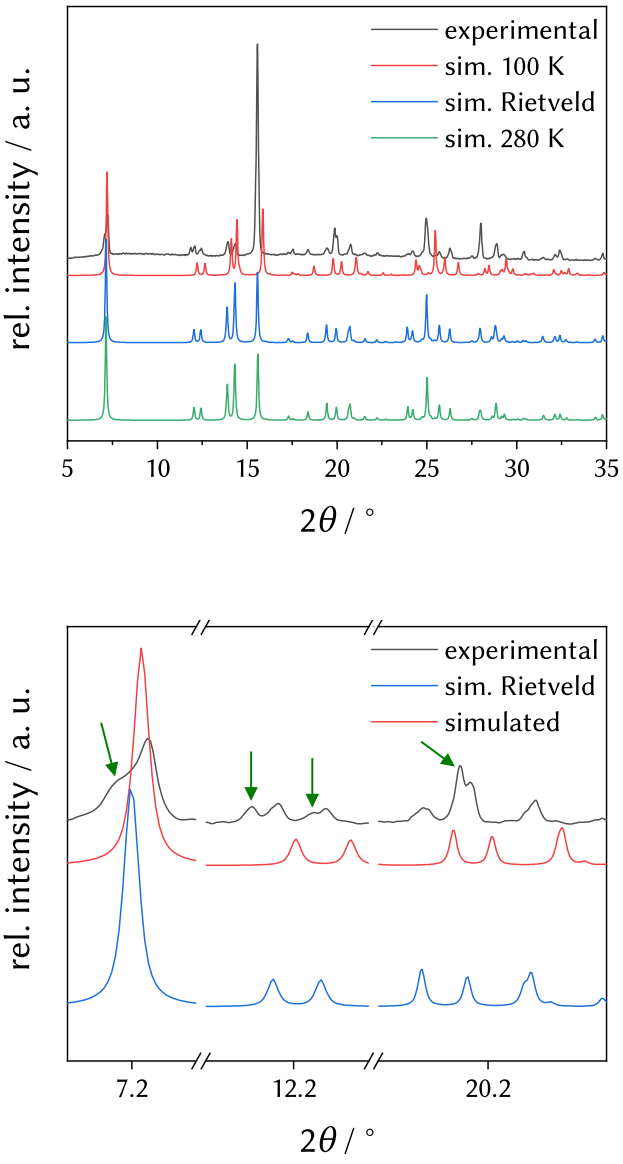


Figure S1. Simulated (100 K and 280 K), Rietveld refined and experimental powder X-ray diffractograms of **1** (top). Three reflections that cannot be assigned to **1** have been marked with green arrows (bottom).

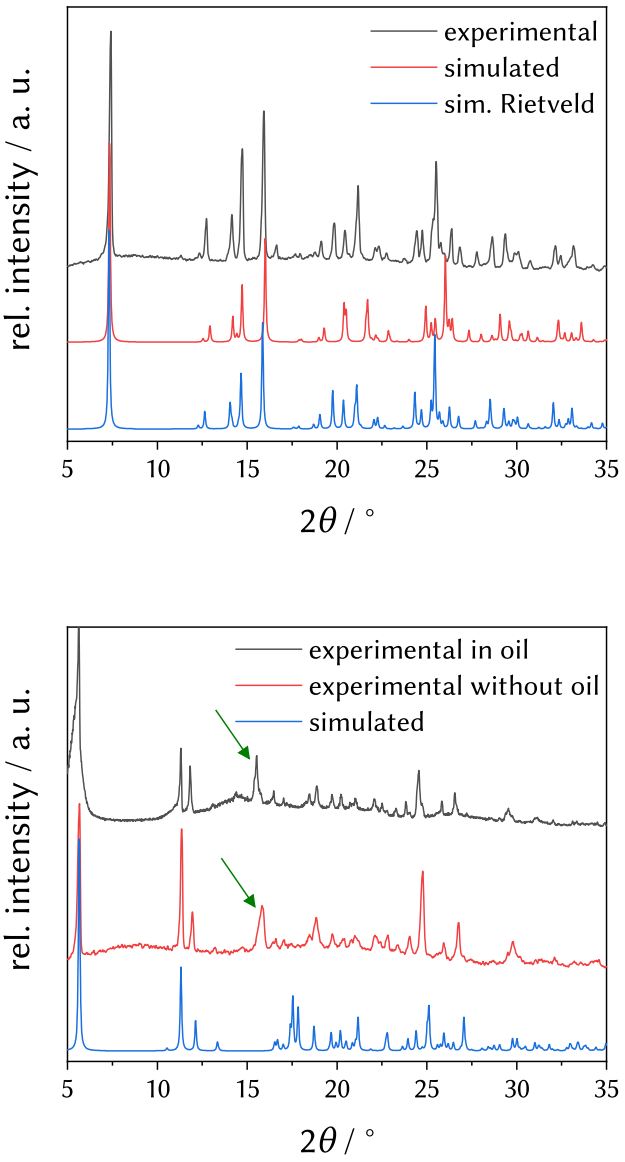


Figure S2. Simulated and experimental powder X-ray diffractograms of **2** (top). Simulated and two experimental powder X-ray diffractograms (with and without oil) of **3** (bottom). The most obvious discrepancies have been marked with an arrow.

2. Single Crystal Details and Convergence Results

Table S1. Crystal and refinement data for **1**, **2** and **3** · 2 MeCN measured at 100(2) K.

Compound	**1**	**2**	**3** · 2 MeCN
Empirical formula	$C_{22}H_{32}AgF_6N_4O_4P$	$C_{11}H_{16}AuClN_2O_2$	$C_{26}H_{36}Au_2Cl_2CuN_6O_4$
Moiety formula	$C_{22}H_{32}AgN_4O_4$, PF_6	$C_{11}H_{16}AuClN_2O_2$	$C_{22}H_{30}Au_2Cl_2CuN_4O_4$, $2\,C_2H_3N$
M_r / g mol^{-1}	669.35	440.67	1024.98
Crystal description	colorless block	colorless block	light blue plate
Crystal size / mm^3	0.14 × 0.12 × 0.12	0.14 × 0.08 × 0.08	0.05 × 0.05 × 0.01
Crystal system	orthorhombic	orthorhombic	monoclinic
Space group (No.)	*Pbca* (61)	*Pbca* (61)	$P2_1/c$ (14)
a / Å	8.9654(4)	8.7023(16)	15.627(3)
b / Å	12.5295(8)	12.463(2)	9.939(2)
c / Å	24.5295(3)	24.052(4)	10.725(2)
β / °	90	90	90.726(3)
V / Å^3	2755.4(2)	2608.7(8)	1665.5(6)
Z	4	8	2
ϱ_{calc} / g cm^{-3}	1.614	2.244	2.044
μ / mm^{-1}	0.865	11.475	9.619
λ / Å	0.71073	0.71073	0.71073
$\sin(\theta_{max})/\lambda$ / Å	0.91	0.72	0.63
total/unique refl.	83859/8597	37759/4015	19552/3413
observed refl.	3971	3154	2836
No. of parameters	180	162	193
R_{int}	0.1668	0.0773	0.0617
$R(I > 2\sigma(I))$	0.0510	0.0338	0.0377
wR_2 (all data)	0.1406	0.0739	0.0986
S (all data)	0.927	1.050	1.032
ρ_{min}/ρ_{max} / e Å^{-3}	–0.910/3.456	–1.377/1.623	–1.618/1.735
CCDC #	2181634	2181635	2181636