

Supplementary Materials: Argentophilic Interactions in Two Ag^I Complexes of 3-(2-(Pyridin-4-yl)ethyl)pentane-2,4-dione, a Promising Ditopic Ligand

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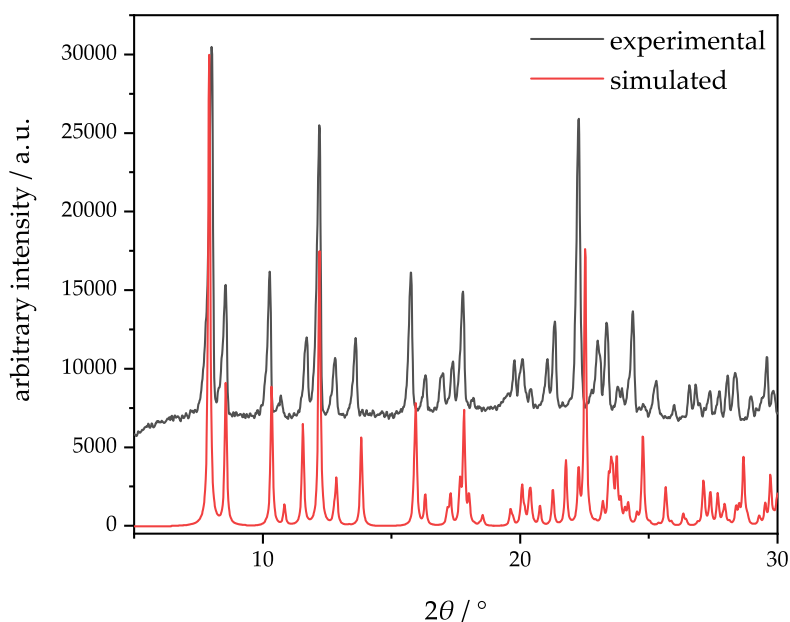


Figure S1. Experimental and simulated X-ray powder diffractogram of **1**. The simulation is based on the single crystal experiment conducted at 100 K whereas the experimental pattern was registered at room temperature, thus leading to slightly smaller 2θ values for the latter.

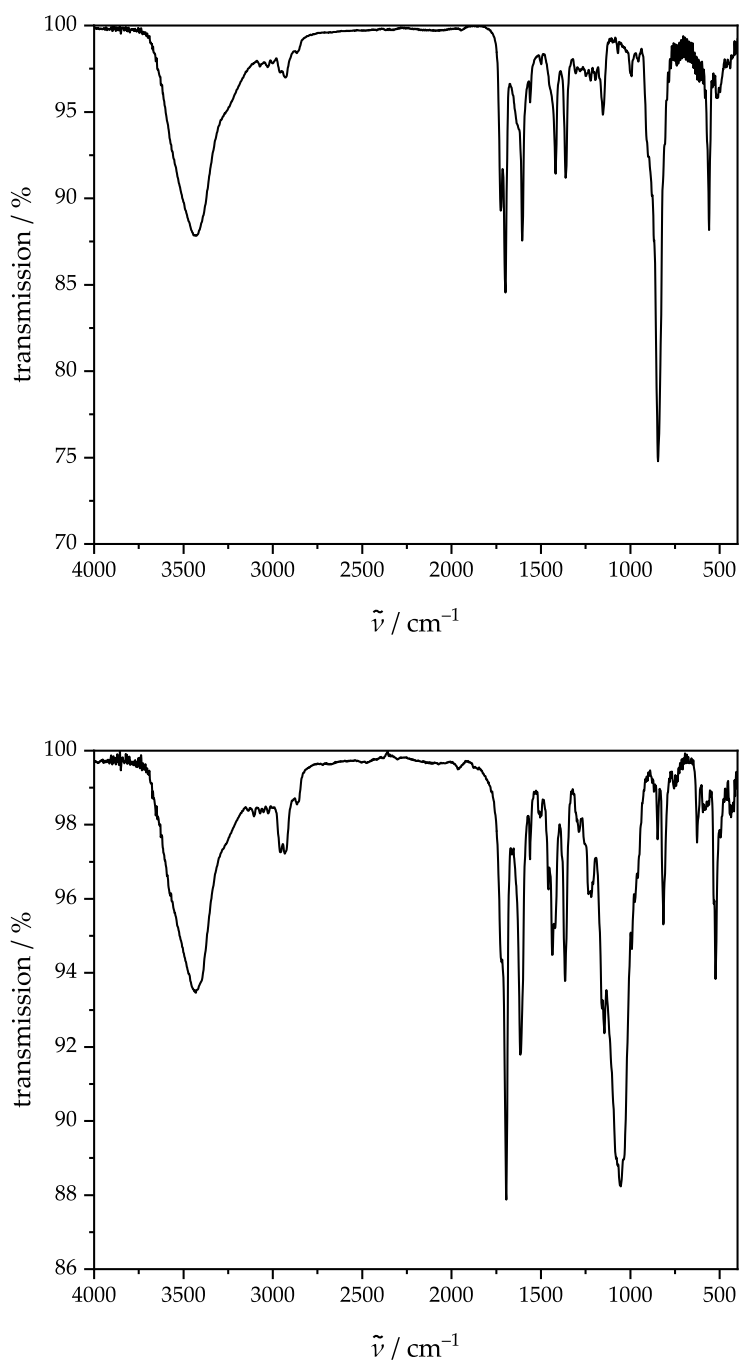


Figure S2. IR spectra of **1** (top) and **2** (bottom).

Table S1. Crystal data, data collection parameters and refinement results for **1**.

Crystal data		
Composition	$\text{C}_{24}\text{H}_{30}\text{AgF}_6\text{N}_2\text{O}_4\text{P}$	$\text{C}_{28}\text{H}_{38}\text{AgBF}_4\text{N}_2\text{O}_6$
Space group (No.)	$P2_1/c$ (14)	$P\bar{1}$ (2)
Crystal system	monoclinic	triclinic
$a / \text{\AA}$	10.8000(16)	11.1270(11)
$b / \text{\AA}$	16.310(2)	14.8723(14)
$c / \text{\AA}$	16.006(2)	20.5106(19)
$\alpha / ^\circ$		77.897(2)
$\beta / ^\circ$	107.103(4)	74.931(2)
$\gamma / ^\circ$		75.966(2)
$V / \text{\AA}^3$	2694.7(7)	3140.5(5)
Z	4	4
$\rho_{\text{calc}} / \text{g cm}^{-3}$	1.635	1.466
μ / mm^{-1}	0.882	0.707
Data collection parameters		
T / K	100(2)	100(2)
Crystal size / mm	$0.59 \times 0.09 \times 0.06$	$0.25 \times 0.15 \times 0.15$
$\theta_{\text{min}} / \theta_{\text{max}} / ^\circ$	2.38/19.14	1.43/27.63
No. of reflections	30097	42177
Independent reflections	4940	14589
Observed reflections	3516	11324
Absorption correction	multi-scan	multi-scan
Refinement results		
Reflections in refinement	4940	14589
Parameters in refinement	347	658
Restraints	0	0
$R_1 / \%$	4.76	3.85
$wR_2 / \%$	10.77	10.79
GOF	1.026	1.080
$\rho_{\text{min}} / \rho_{\text{max}} / e \text{\AA}^{-3}$	-0.45/0.49	-0.63/1.81