Supporting Information

(5 pages)

Exploring the co-crystallization of kojic acid with copper(II), silver (I), zinc(II) and gallium(III) for potential antibacterial applications.

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Structural characterization via X-ray diffraction

Table S1. Crystal data and details of measurements for the compounds described in this work (HKA = kojic acid; KA = kojiate anion).

Compound	**$Zn(KA)_2$**	**$Cu(KA)_2$[a]**	**$[Ag(HKA)(NO_3)]\cdot H_2O$**	**$[Ga(KA)_2(OH_2)_2][NO_3]\cdot H_2O$**
Chemical formula	$C_{12}H_{10}O_8Zn$	$C_{12}H_{10}CuO_8$	$C_6H_8AgNO_7\cdot H_2O$	$C_{12}H_{15}GaNO_{14}$
Formula weight	347.57	345.00	330.00	466.97
Temperature (K)	298	298	223	298
Crystal system	Triclinic	Monoclinic	Orthorhombic	Monoclinic
Space group	*P*-1	$P2_1/a$	$Pn2_1/a$	$P2_1/c$
a (Å)	5.1557(5)	15.313(2)	14.4029(5)	11.4594(11)
b (Å)	7.7602(7)	6.805(2)	3.6487(2)	21.4272(16)
c (Å)	7.8702(7)	11.923(2)	17.9803(7)	7.0775(15)
α (°)	94.492(7)	90	90	90
β (°)	108.982(8)	110.158(3)	90	90.157(13)
γ (°)	97.130(7)	90	90	90
V (Å^3)	293.08(5)	1171(3)	944.90(7)	1737.8(4)
Z	1	4	4	4
F(000)	176.0	700.0	645.0	948.0
ρ_{calc}(g·cm^{-3})	1.969	1.961	2.320	1.785
Mμ(mm^{-1})	2.137	3.070	2.164	1.662
R_{wp}	---	0.0417	---	---
N_{reflns}, N_{par}	1339, 98	---	1634, 153	3187, 266
R1 [F_0^2, I>2σ(I)]	0.0375	---	0.0362	0.0847
wR2 (all data)	0.0770	---	0.0591	0.2038

[a] Structural solution from powder data.

Powder X-ray diffraction

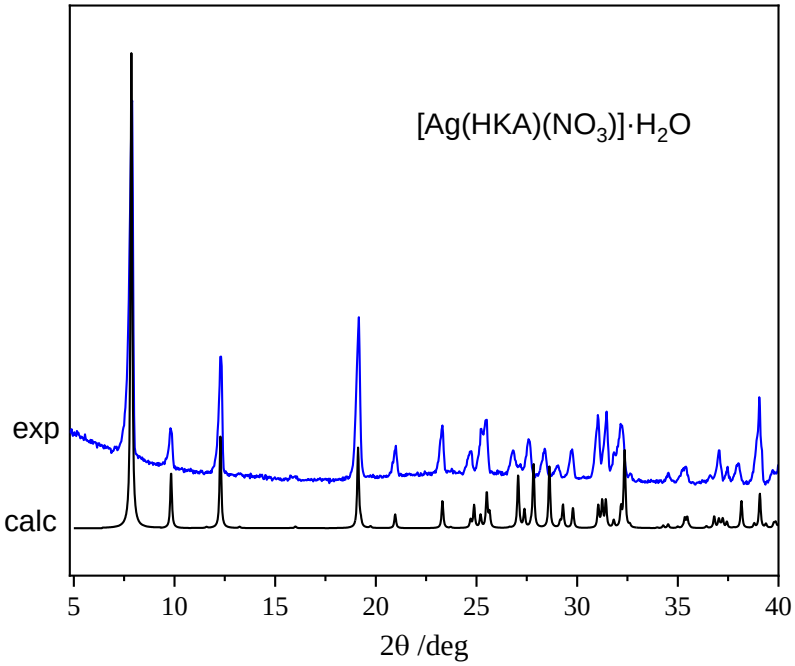

Figure S1: Comparison between the experimental pattern for the ball milling product of the reaction between HKA and $AgNO_3$ (blue line) and the pattern calculated from single crystal data for $[Ag(HKA)(NO_3)]\cdot H_2O$ (black line). Small differences in the peaks positions are due to the difference in the powder data collection temperature (RT) with respect to single crystal (223 K).

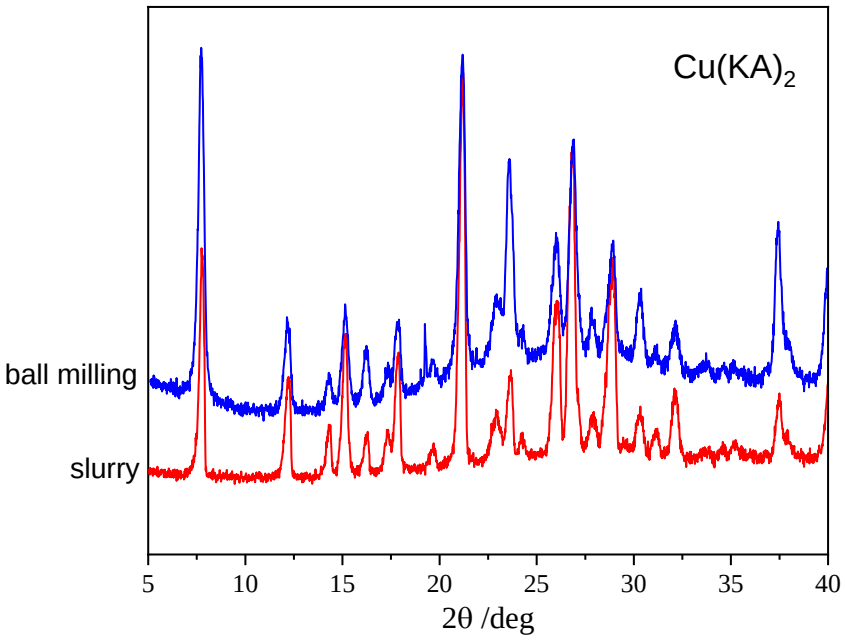

Figure S2: Comparison between XRD patterns for the slurry (red line) and ball milling (blue line) products of the reaction between HKA and $Cu(NO_3)_2$.

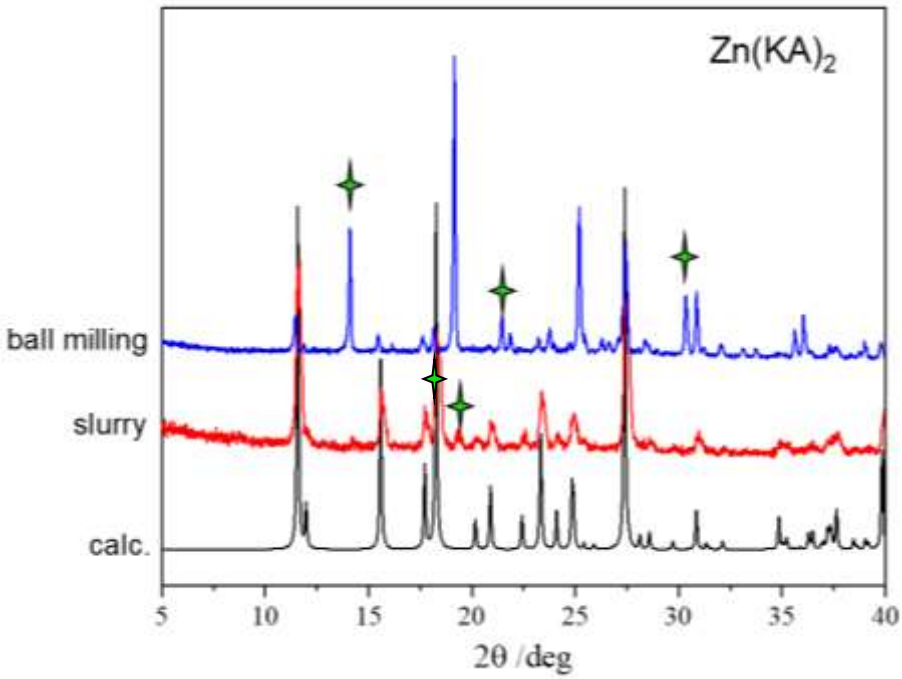

Figure S3: Comparison between the experimental patterns of ball milling (blue line) and slurry (red line) products of the reaction between HKA and $Zn(NO_3)_2$, and the pattern calculated from $Zn(KA)_2$ single crystal data (black line). Green stars indicate the presence of unreacted HKA (almost absent in the slurry product).

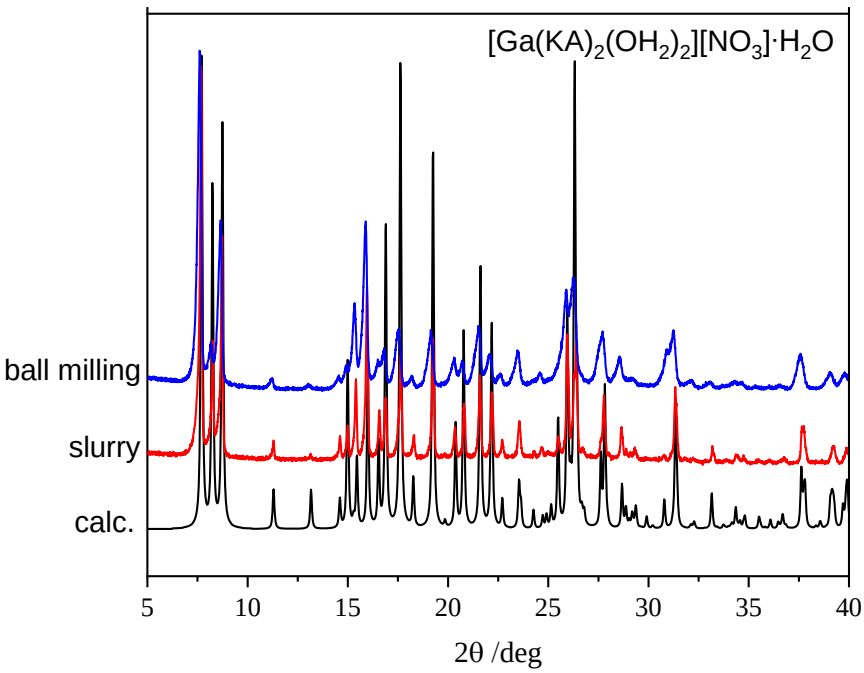

Figure S4: Comparison between the experimental patterns for the ball milling (blue line) and slurry (red line) products of the reaction between HKA and $Ga(NO_3)_3$, and the pattern calculated from single crystal data for $[Ga(KA)_2(OH_2)_2][NO_3]\cdot H_2O$ (black line).

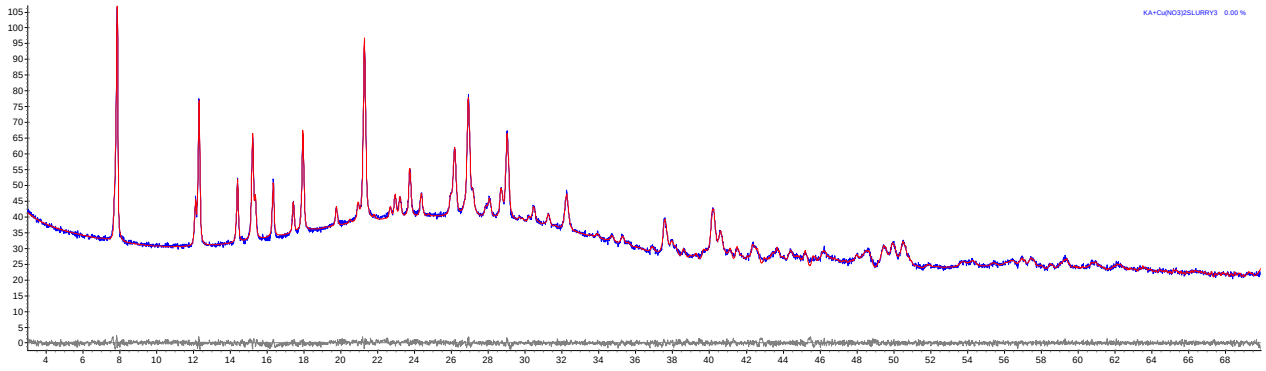

Figure S5: Pawley refinement plots for $Cu(KA)_2$.

Thermogravimetric analysis (TGA)

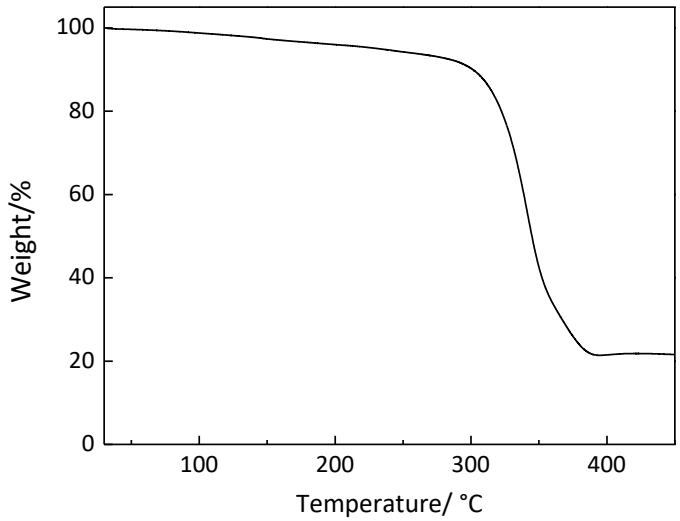

Figure S6: TGA trace for the product of the slurry reaction between HKA and $Cu(NO_3)_2$.