

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 = kojate anion).

Compound	Zn(KA) ₂	Cu(KA) ₂ ^a	[Ag(HKA)(NO ₃)]·H ₂ O	[Ga(KA) ₂ (OH ₂) ₂][NO ₃]·H ₂ O
Chemical formula	C ₁₂ H ₁₀ O ₈ Zn	C ₁₂ H ₁₀ CuO ₈	C ₆ H ₈ AgNO ₇ ·H ₂ O	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	<i>P</i> -1	<i>P</i> 2 ₁ / <i>a</i>	<i>P</i> n2 ₁ / <i>a</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> (Å)	5.1557(5)	15.313(2)	14.4029(5)	11.4594(11)
<i>b</i> (Å)	7.7602(7)	6.805(2)	3.6487(2)	21.4272(16)
<i>c</i> (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
<i>V</i> (Å ³)	293.08(5)	1171(3)	944.90(7)	1737.8(4)
<i>Z</i>	1	4	4	4
<i>F</i> (000)	176.0	700.0	645.0	948.0
ρ_{calc} (g·cm ⁻³)	1.969	1.961	2.320	1.785
<i>M</i> μ (mm ⁻¹)	2.137	3.070	2.164	1.662
<i>R</i> _{wp}	---	0.0417	---	---
<i>N</i> _{refl} , <i>N</i> _{par}	1339, 98	---	1634, 153	3187, 266
<i>R</i> 1 [<i>F</i> _o ² , <i>I</i> > 2σ(<i>I</i>)]	0.0375	---	0.0362	0.0847
<i>wR</i> 2 (all data)	0.0770	---	0.0591	0.2038

^a Structural solution from powder data.

Powder X-ray diffraction

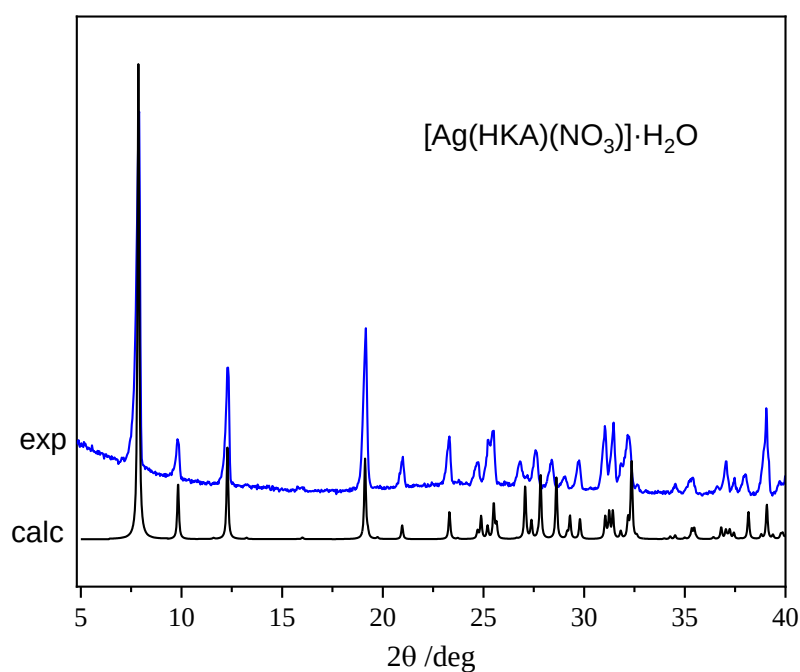


Figure S1: Comparison between the experimental pattern for the ball milling product of the reaction between HKA and AgNO_3 (blue line) and the pattern calculated from single crystal data for $[\text{Ag}(\text{HKA})(\text{NO}_3)] \cdot \text{H}_2\text{O}$ (black line). Small differences in the peaks positions are due to the difference in the powder data collection temperature (RT) with respect to single crystal (223 K).

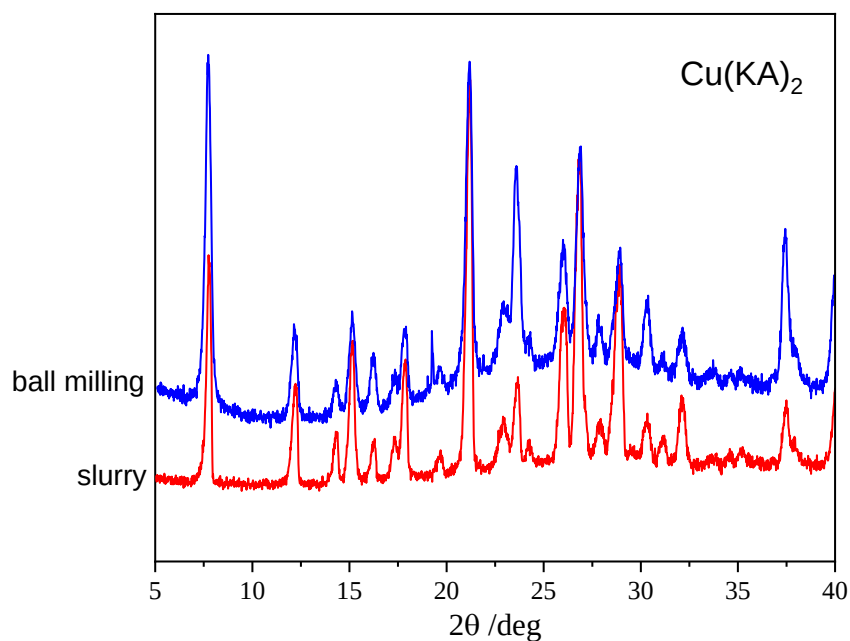


Figure S2: Comparison between XRD patterns for the slurry (red line) and ball milling (blue line) products of the reaction between HKA and $\text{Cu}(\text{NO}_3)_2$.

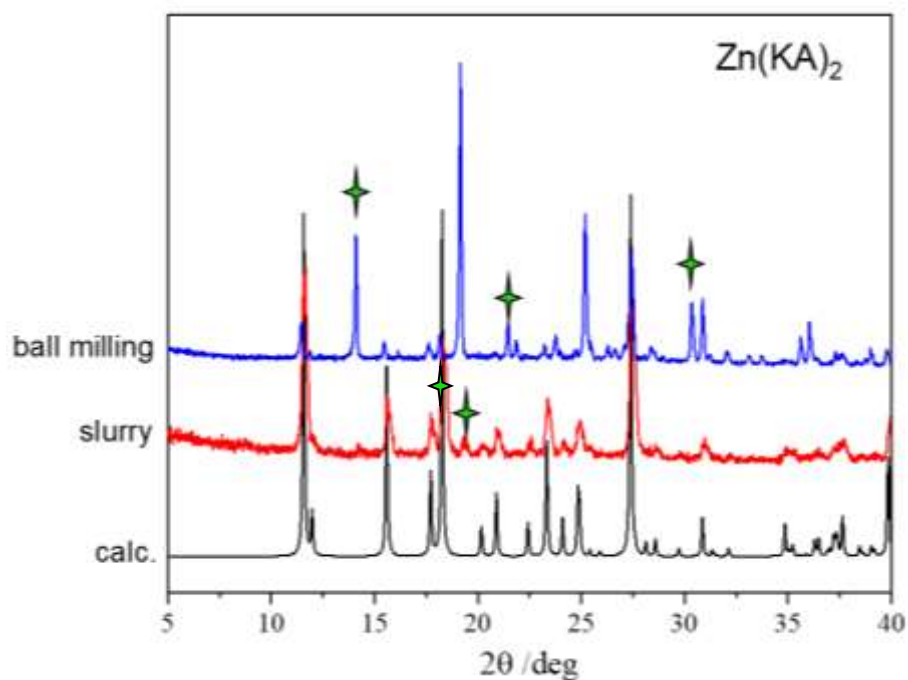


Figure S3: Comparison between the experimental patterns of ball milling (blue line) and slurry (red line) products of the reaction between HKA and $\text{Zn}(\text{NO}_3)_2$, and the pattern calculated from $\text{Zn}(\text{KA})_2$ single crystal data (black line). Green stars indicate the presence of unreacted HKA (almost absent in the slurry product).

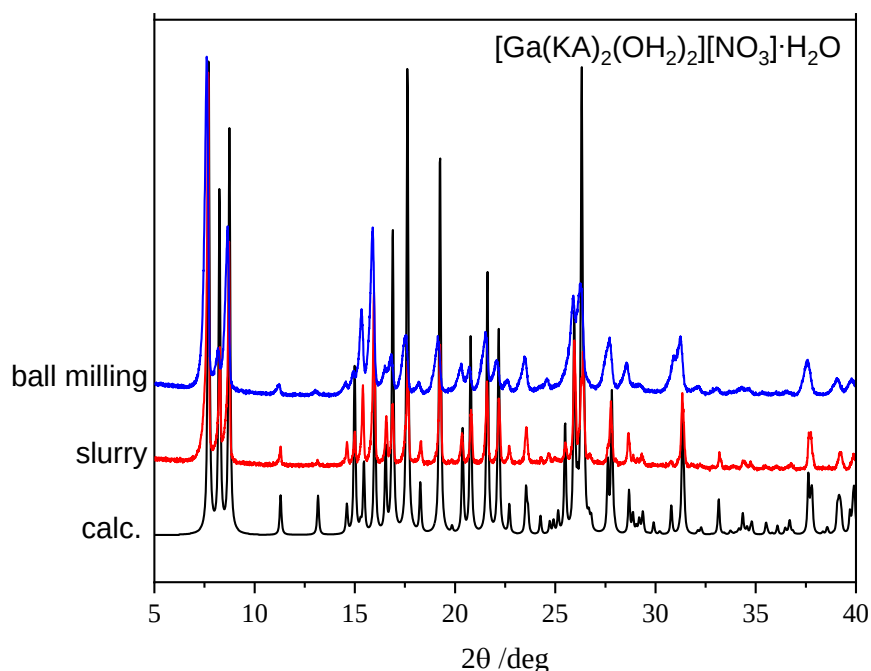


Figure S4: Comparison between the experimental patterns for the ball milling (blue line) and slurry (red line) products of the reaction between HKA and $\text{Ga}(\text{NO}_3)_3$, and the pattern calculated from single crystal data for $[\text{Ga}(\text{KA})_2(\text{OH}_2)_2][\text{NO}_3] \cdot \text{H}_2\text{O}$ (black line).

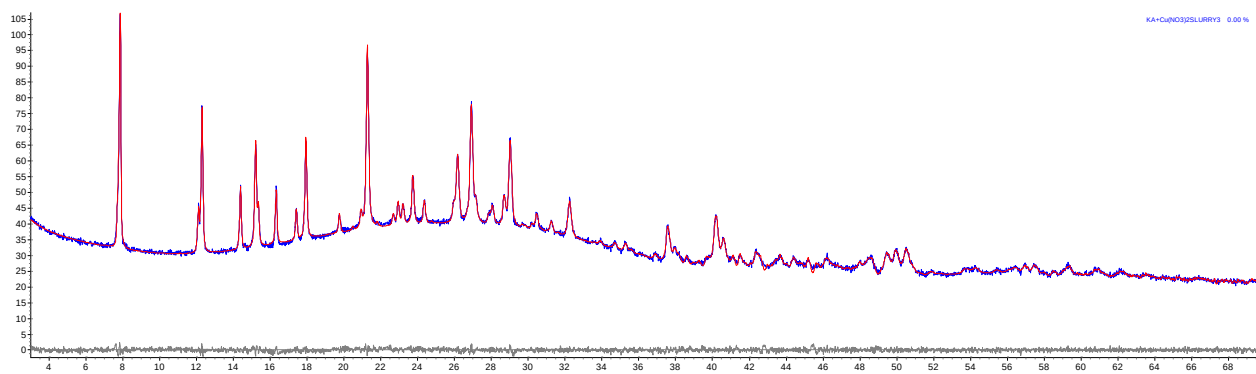


Figure S5: Pawley refinement plots for Cu(KA)_2 .

Thermogravimetric analysis (TGA)

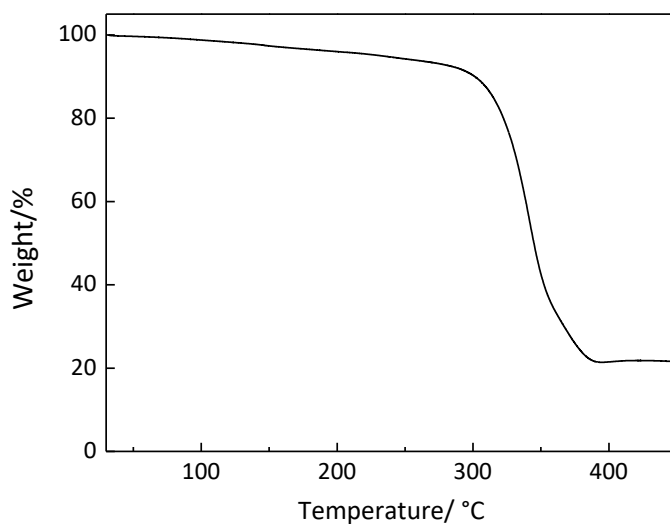


Figure S6: TGA trace for the product of the slurry reaction between HKA and $\text{Cu(NO}_3)_2$.