

Supporting Information

What roles do alkali metal ions play in pathological crystallization of uric acid?

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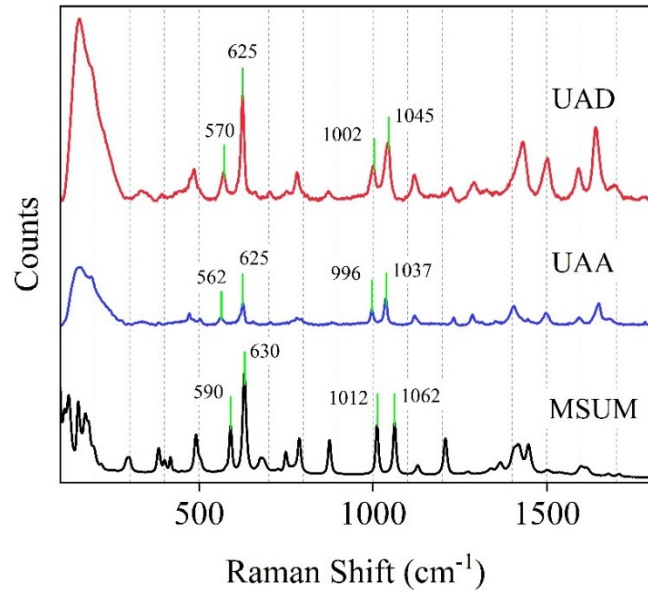


Figure 1. Raman spectrum of UAD, UAA and MSUM powders.

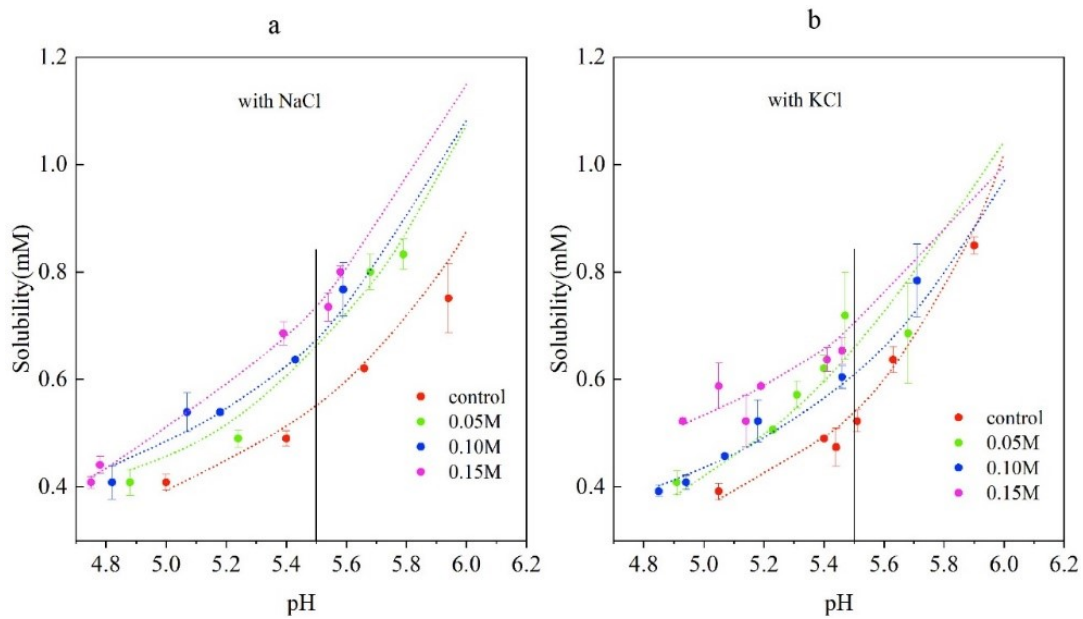


Figure 2. Solubility of UAD in buffer (pH 4.5-6.0) in presence of different concentration (a) NaCl and (b) KCl under 25°C. The black lines represent pH is 5.5.

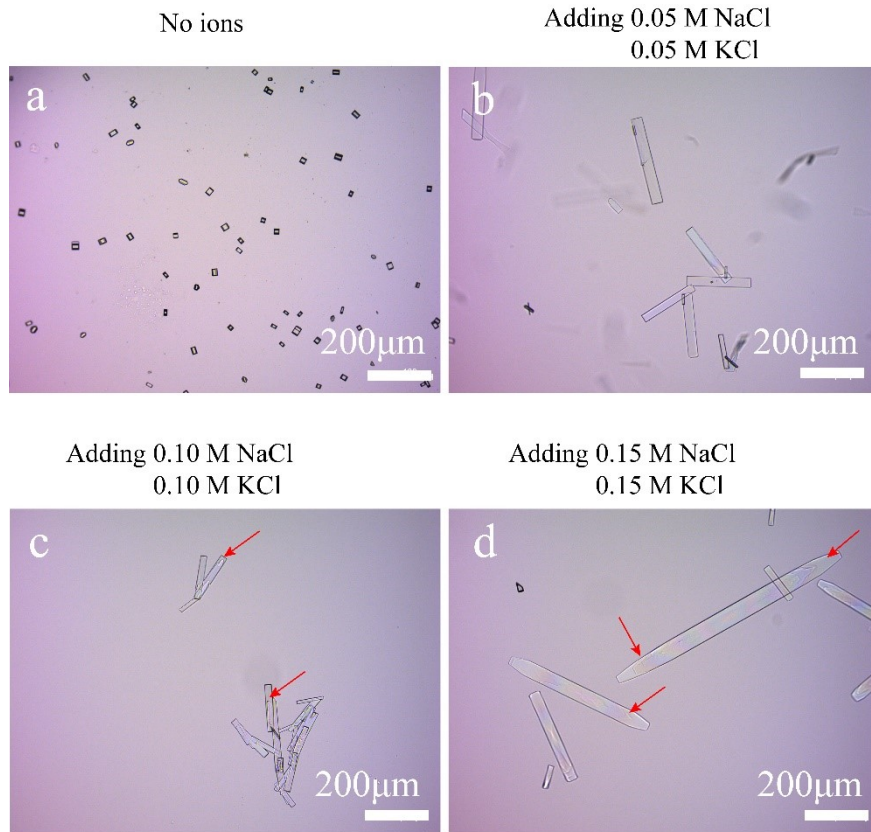


Figure 3. Crystal morphology of UAD in solution with different concentration NaCl and KCl by optical microscopy: (a) crystals from 4 mM UA solution without ions; (b) crystals from 4 mM UA solution with 0.05 M NaCl and 0.05M KCl; (c) crystals from 4 mM UA solution with 0.10 M NaCl and 0.10 M KCl; (d) crystals from 4 mM UA solution with 0.15 M NaCl and 0.15 M KCl.

Table 1. The relative intensity of the characteristic peaks of the PXRD patterns of UAD crystals in the absence and presence of ions corresponding to the different planes.

Crystal planes	Blank UAD	With NaCl	With Na ₂ SO ₄	With KCl	With K ₂ SO ₄
(002)	1.0	1.0	1.0	1.0	1.0
(011)	0.017	0.092	0.052	0.092	0.066
(102)	0.036	0.171	0.120	0.221	0.121
(004)	0.063	0.088	0.090	0.095	0.109
(112)	0.031	0.130	0.108	0.179	0.122
(10-4)	0.038	0.124	0.101	0.157	0.136
(210)	0.081	0.497	0.307	0.856	0.327

Table 2. Adsorption energy^a of ions on different crystal planes of UAD.

additives/planes	(001)	(010)	(011)	(100)	(102)
NaCl	-1.60	-1.39	-1.03	-1.37	-1.35
Na ₂ SO ₄	-3.32	-2.42	-2.15	-2.70	-2.26
KCl	-1.57	-1.33	-1.11	-1.52	-1.27
K ₂ SO ₄	-3.06	-2.24	-2.00	-2.51	-2.09

^a represent the unit is *kcal/mol/nm²*.