

Supporting Information

Insight into the role of hydrochloric acid in the thermodynamics and nucleation kinetics behavior of Arbidol hydrochloride monohydrate from Metastable Zone Widths

Ting Wen ^{a,‡}, Hairong Wang ^{a,‡,*}, Chunrong Li, Jikun Xu ^{a,*}, Chuntao Zhang ^{a,*}

^aSchool of Chemistry and Chemical Engineering, Wuhan University of Science and Technology, Wuhan Hubei 430081, P. R. China

[‡] These authors contributed equally to this work and should be regarded as co-first authors.

* Corresponding author: Hairong Wang, Jikun Xu, and Chuntao Zhang

E-mail: wanghairong@wust.edu.cn (H. Wang) ; jkxu@wust.edu.cn (J. Xu) and zhangchuntao@wust.edu.cn (C. Zhang)

Table S1 Regression results and model parameters of modified Apelblat model of AHM in three solvent systems

ω (HCl)	model parameters			100ARD	10 ³ RMSD
	<i>A</i>	<i>B</i>	<i>C</i>		
0	-400.82	15035.16	60.57	1.37	0.12
0.25%	-158.42	3526.83	24.76	0.54	0.040
0.5%	-206.15	5483.30	31.96	0.93	0.066

Table S2 Comparison of Experimental and Predicted Induction Time of AHM at 303.15 K

supercooling		$\omega(\text{HCl})=0\%$		supercooling		$\omega(\text{HCl})=0.25\%$	
ΔT	$t_{\text{ind}}^{\text{exp}}(\text{s})$	$t_{\text{ind}}^{\text{cal}}(\text{s})$	RD	ΔT	$t_{\text{ind}}^{\text{exp}}(\text{s})$	$t_{\text{ind}}^{\text{cal}}(\text{s})$	RD
3.2	4457	3991	11.68	3.3	1754	1876	6.50
3.6	2490	2684	7.21	3.8	962	1155	16.68
4.2	1840	1597	15.25	4.1	806	889	9.34
4.7	1251	1093	14.46	4.7	494	556	11.11
5.3	940	729	28.92	5.2	460	393	17.20
5.8	631	538	17.25	5.6	358	304	17.69
6.4	499	386	29.19	6.1	321	227	41.62

$t_{\text{ind}}^{\text{exp}}$ and $t_{\text{ind}}^{\text{cal}}$ denote the experimental induction time and calculated by Kubota theory, respectively.

Table S3 *T*-test of $(T_0/T_{\max})^2 / (T_0 - T_{\max})$ and $\ln(R/T_0(T_0 - T_{\max}))$ in the aqueous THF system free of HCl

	Std. Error Mean	95% Confidence Interval of the Difference		R_t	Significance(<i>P</i>)
		Lower	Upper		
		303.15 K	1.9890		
313.15 K	2.9435	-41.7879	-25.4430	-0.9991	0.0000339
323.15 K	5.6386	-60.4453	-29.1350	-0.9980	0.0001093

Significance Level $\alpha=0.05$

R_t represents the significance test of correlation coefficient, which becomes a trend of negative correlation.

Table S4 *T*-test of $(T_0/T_{\max})^2/(T_0-T_{\max})$ and $\ln(R/T_0(T_0-T_{\max}))$ in different hydrochloric acid contents

Saturation Temperature	Std. Error Mean	95% Confidence Interval of the Difference		R_t	Significance(<i>P</i>)
		Lower	Upper		
303.15 K	3.6039	-46.0304	-26.0181	-0.9985	0.00006973
	2.4756	-36.9025	-23.1556	-0.9985	0.00007012
	1.9890	-32.2673	-21.2225	-0.9957	0.0003367
313.15 K	6.5822	-63.0119	-26.4618	-0.9953	0.0003919
	3.9063	-48.3567	-26.6652	-0.9953	0.0003885
	2.9435	-41.7879	-25.4430	-0.9991	0.00003388
323.15 K	22.8293	-149.4814	-22.7126	-0.9954	0.0003691
	10.6330	-84.9824	-25.9383	-0.9963	0.0002722
	5.6386	-60.4453	-29.1350	-0.9980	0.0001093

Significance Level $\alpha=0.05$

R_t represents the significance test of correlation coefficient, which becomes a trend of negative correlation.

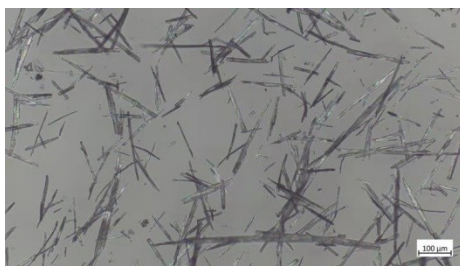


Fig.S1 SEM of the powder product of AHM re-crystallized from water and THF binary-solvents

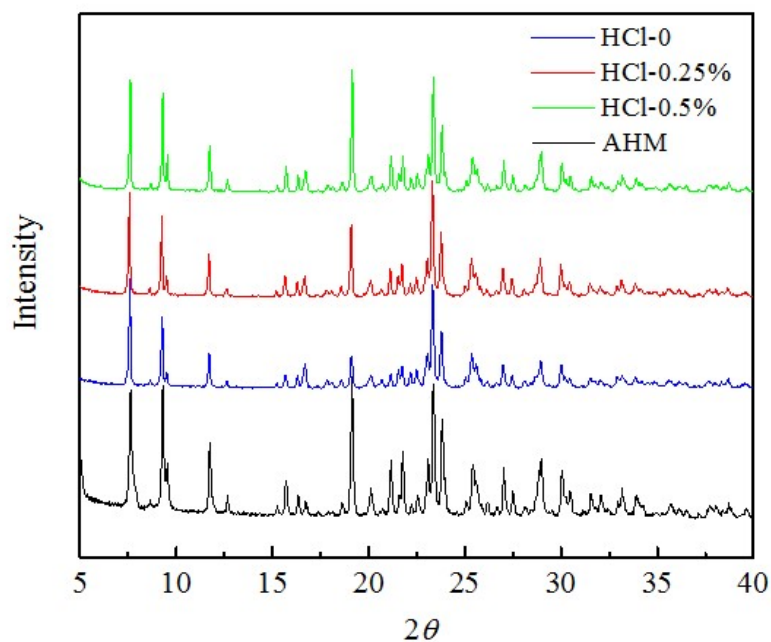


Fig.S2 PXRD patterns of the powder product of AHM re-crystallized from water and THF binary-solvents with different HCl contents

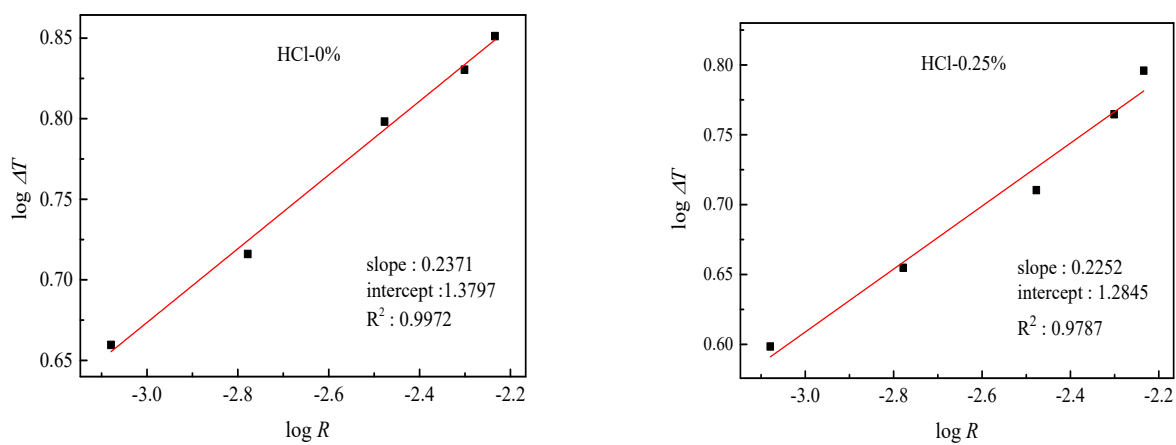


Fig.S3 Slopes and intercepts estimated from MSZW data at 303.13K, using Kubota's theory.