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Supporting information

Induction time

Experimental induction time results are usually evaluated by plotting lnt_{ind} versus $T^{-3}(lnS)^{-2}$ for determination of the solid-liquid interfacial free energy, σ , from the slope, B, of the correlated linear line,

$$B = \frac{16\pi\sigma^3 v^2}{3k^3} \tag{1}$$

$$\sigma = \left(\frac{3k^{3}B}{16\pi\nu^{2}}\right)^{\frac{1}{3}}$$
(2)

Knowing the interfacial energy allows for calculation of the critical free energy, ΔG_c , of the nucleation and the radius, r_c , of the critical nucleus.



Figure: Determination of the interfacial energy and pre-exponential factor from the linear correlation (dashed line) i.e. $lnt_{ind \text{ vs. }} T^{-3} (lnS)^{-2}$.



Figure: Experimental MSZWs and estimated MSZWs from induction time experiments of isonicotinamide in ethanol and paracetamol in ethanol.

Optimization method:

For example in optimization of BP in ethanol, N from 0 to 1000000, ten big steps ($\Delta N = 100000$, $\Delta \ln AV = 1$) are used to do the first step of the optimization, and the maximum and minimum value of N and AV from the best 3 fitting results are used as the new range to apply ten small steps ($\Delta N = 10000$, $\Delta \ln AV = 0.1$) to find the best fitting result. The N and AV results are shown in the table.

	Optimization conditions	F _{opti}	N	AV	σ
Experimental	-	8.4691	1.10	0.014	1.134
Estimated	At 4.0K/hour	<0×10-7	1.12	0.100	1.141
	At 6.0K/hour	<0×10-7	0.88	0.050	1.053
	At 12.0K/hour	<0×10-7	0.74	0.027	0.994
	At 15.0K/hour	<0×10-7	1.33	0.165	1.208
	At 20.0K/hour	<0×10-7	1.14	0.074	1.147

Table: Estimated interfacial energies and pre-exponential factors from optimizing equation (Eqn. 6) of butyl paraben in ethanol

From the Eqn. 2, the critical nucleation potential of ascorbic acid in water is 89.55 (kJ/mol)³, and AV is 0.029 s⁻¹ (Table 2). At constant cooling rate 18.0 K/hour (0.005 K/sec), the temperature is equal to $307.98 - 0.005n\Delta t$ K at time $n\Delta t$ with unit of second. If the time step, Δt , is 1 second, combining the solubility equation, $lnx = 21.123T^{-1} - 11.845 + 0.028T$, with Eqn. 5, the accumulated nucleation potential of every short time step (one second) during the cooling process can be calculated:

$$\sum_{n=1}^{m} \Delta N = \sum_{n=1}^{m} \frac{3.088 \times 10^{12} n}{exp^{[m]} (\frac{51953964}{(307.98 - 0.005n)^3 \left[0.069 - \frac{21.12}{307.98 - 0.005n} + 2.32 \times 10^{-5}n \right]^2})}$$