Supplementary material

Probing the Influence of Electronic Effects of Organic Additives on the Morphology of Sodium Chloride Crystals: A Combined Experimental and Computational Study

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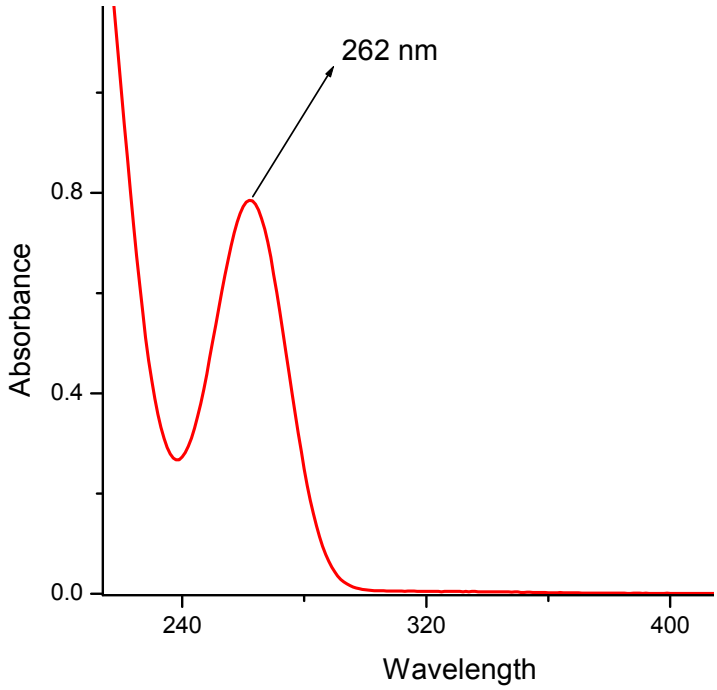
(1) Thioformamide, IR and UV.

(b) FTIR Spectra for Thioformamide (ν, cm^{-1}): 855, 945, 1,095, 1,140, 1,232, 1,300, 1,315, 1,400, 1,465, 1,505, 1,737, 2,880, 2,930

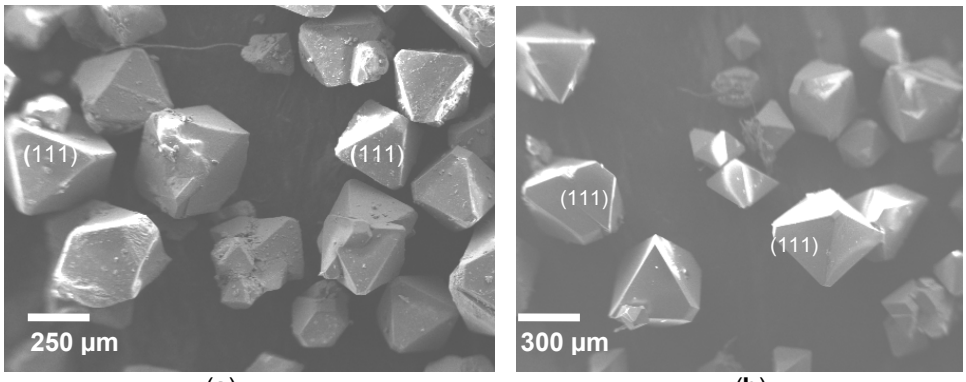
(c) UV Absorption spectrum of Thioformaide in methanol.



(2) Crystallization process of urea and formamide with NaCl:

(**I**) Urea was added in the saturated solution of NaCl in three different concentrations namely 20, 25 and 30 wt.% (w/w). After complete dissolution of the solid additive, the clear solutions were filtered and transferred to glass beaker of similar capacity. Crystallization was carried out at ambient conditions where the temperature was maintained at 25°C (Figure S1: a).

(**II**) To a saturated solution of NaCl, 20, 25 and 30 wt.% (w/w) of formamide as additive was added in a glass beaker of 10 ml capacity in three different set of crystallization. After complete homogenization of the solution, the mixture was filtered and kept in a separate beaker of similar volumetric capacity. Crystallization was carried out at ambient conditions where the temperature was maintained at 25°C (Figure S1: b).



(**a**) (**b**)

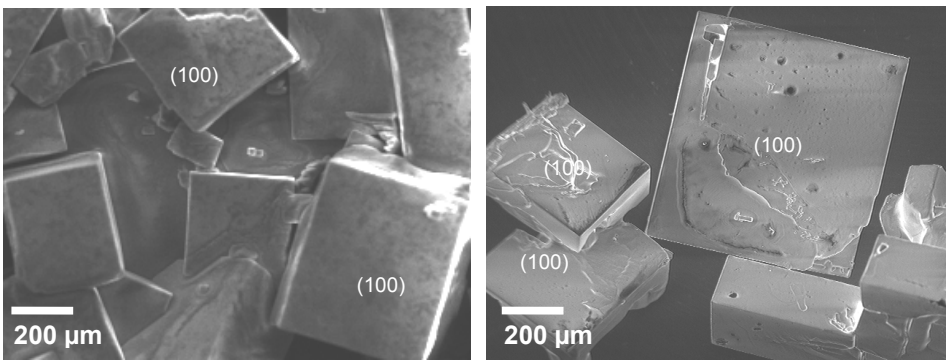
Figure S1: (a) Ex situ SEM image of NaCl crystals grown from urea solution; (b) Ex situ SEM image of NaCl crystals grown from fromamide solution.

(**III**) 5 ml saturated NaCl solution was taken in a glass beaker of 10 ml capacity. 40 wt.% (w/w) thiourea was added as a habit modifier in the saturated solution of NaCl. After complete homogenization of the solution, the mixture was filtered and kept in a separate beaker of similar volumetric capacity. Crystallization was carried out at ambient conditions where the temperature was maintained at 25°C.

(**IV**) 5 ml saturated NaCl solution was taken in a glass beaker of 10 ml capacity. 40 wt.% (w/w) thioformamide was added as a habit modifier in the saturated solution of NaCl. After complete homogenization of the solution, the mixture was filtered and kept in a separate beaker of similar volumetric capacity. Crystallization was carried out at ambient conditions where the temperature was maintained at 25°C.

(**V**) 5 ml saturated NaCl solution was taken in a glass beaker of 10 ml capacity. 50 wt.% (w/w) thiourea was added as a habit modifier in the saturated solution of NaCl. After complete homogenization of the solution, the mixture was filtered and kept in a separate beaker of similar volumetric capacity. Crystallization was carried out at ambient conditions where the temperature was maintained at 25°C (Figure SII a).

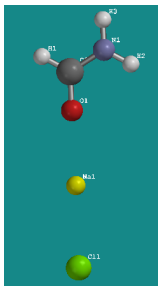
(**VI**) 5 ml saturated NaCl solution was taken in a glass beaker of 10 ml capacity. 50 wt.% (w/w) thioformamide was added as a habit modifier in the saturated solution of NaCl. After complete homogenization of the solution, the mixture was filtered and kept in a separate beaker of similar volumetric capacity. Crystallization was carried out at ambient conditions where the temperature was maintained at 25°C (Figure SII b).



(a) (b)

Figure SII: (a) Ex situ SEM image of NaCl crystals grown from thiourea solution; (b) Ex situ SEM image of NaCl crystals grown from thioformamide solution.

(**3**) Morokuma decomposition analysis:



RHF/6-31G* Level	Energies in kcal/mol.
Electrostatic Energy (Es)	-42.0
Exchange repulsion Energy (Ex)	25.4
Polarization Energy (PL)	-21.7
Charge transfer energy (CT)	-6.9
High order Coupling Energy	13.0
Total Interaction Energy	-30.9